



Tara Government College, Sangareddy (A)

DEPARTMENT OF CHEMISTRY

COURSES HAVING FOCUS ON

EMPLOYABILITY/ENTREPRENEURSHIP/SKILL DEVELOPMENT

B.Sc.-CHEMISTRY:

SEMESTER	COURSE	TYPE	HOURS	CREDITS	MARKS		
					CIA	Exam	Total
Sem - III	SEC- 1 (Safety Rules in chemistry Laboratory and Lab Reagents)	Theory	30	2	10	40	50
	SEC -2 (Remedial methods for pollution, drinking water and Soil fertility)	Theory	30	2	10	40	50
Sem - IV	SEC- 3 (Materials and their Applications)	Theory	30	2	10	40	50
	SEC -4 (Chemistry of Cosmetics and Food Processing)	Theory	30	2	10	40	50
Sem - V	Chemistry – V	Theory	60	4	30	70	100
	Chemistry – V	Practical	45	1	NA	25	25
	GE (Chemistry of Cosmetics, Food processing, Drug and Pharmaceuticals)	Theory	60	4	30	70	100
Sem - VI	Chemistry – VI	Theory	60	4	30	70	100
	Chemistry – VI	Practical	45	1	NA	25	25
	Advanced Chemistry (OR)	Theory	60	4	30	70	100
	Project work	Practical		4	NA	NA	100

CERTIFICATE COURSE:

SEMESTER	COURSE	TYPE	HOURS	CREDITS	MARKS		
					CIA	Exam	Total
Sem – V/VI	Certificate Course on “ Concepts and Analytical Techniques in Pharmaceutical Chemistry and Organic Synthesis”	Theory	30	2	20	30	50
		Practical	30	2	NA	30	30
		Project	NA	1	NA	20	20

M.Sc.-ORGANIC CHEMISTRY:

SEMESTER	COURSE	TYPE	HOURS	CREDITS	MARKS		
					CIA	Exam	Total
Sem -I	Paper- IV CH104 Analytical Techniques and Spectroscopy- I	Theory	60	4	30	70	100
	Paper CH 151: Inorganic chemistry Lab course	Practicals	6hr/Week	3	NA	75	75
	Paper CH 152: Organic Chemistry Lab course	Practicals	4hr/Week	2	NA	50	50
	Paper CH153: Physical Chemistry Lab course	Practicals	6hr/Week	3	NA	75	75
Sem - II	Paper- IV CH204 Analytical Techniques and Spectroscopy- II	Theory	60	4	30	70	100
	Paper CH 251: Inorganic chemistry lab course	Practicals	6hr/Week	3	NA	75	75

	Paper CH 252: Organic Chemistry Lab course	Practicals	6hr/Week	3	NA	75	75
	Paper CH253: Physical Chemistry Lab course	Practicals	4hr/Week	2	NA	50	50
Sem – III	CH(OC)301T Synthetic Reagents, Advanced NMR, Conformational Analysis and ORD	Theory	60	4	30	70	100
	CH(OC)302T Modern Organic Synthesis	Theory	60	4	30	70	100
	CH(OC)303T (CB-1) Bioorganic Chemistry	Theory	60	4	30	70	100
Sem – III	CH(OC)303T (CB-2) Forensic Chemistry and Toxicology	Theory	60	4	30	70	100
	CH(OC)304T (CB-1) Green chemistry and Organic materials	Theory	60	4	30	70	100
	CH(OC)304T (CB-2) Pesticides	Theory	60	4	30	70	100
	CH(OC)351P Synthesis of organic molecules, isolation of natural products & TLC	Practicals	9hr/Week	4	NA	100	100
	CH(OC)352P Separation and identification of organic compounds & Column chromatography	Practicals	9hr/Week	4	NA	100	100
Sem - IV	CH(OC)401T Drug Design and Drug Discovery	Theory	60	4	30	70	100
	CH(OC)402T Drug synthesis and mechanism of action	Theory	60	4	30	70	100
	CH(OC)403T (CB-1) Advanced Heterocyclic Chemistry	Theory	60	4	30	70	100

	CH(OC)403T (CB-2) Polymers , dyes and Pigments	Theory	60	4	30	70	100
	CH(OC)404T (CB-1) Advanced Natural Products	Theory	60	4	30	70	100
	CH(OC)404T (CB-2) Biopharmaceutics and Pharmacodynamics	Theory	60	4	30	70	100
	CH(OC)451P Spectroscopic identification of organic compounds & practice of chemistry software programmes	Practicals	9hr/Week	4	NA	100	100
	CH(OC)452P Synthesis and analysis of drugs	Practicals	9hr/Week	4	NA	100	100
Total				96	2400		

B.Sc. Chemistry II Year Semester-III
Skill Enhancement Course- I (SEC-I) (2 Credits)
Rules in Chemistry Laboratory and Lab Reagents

Unit I: Laboratory Safety Rules and Regulations **15 h (1 hr/week)**

General rules and regulations for lab safety: Minimizing Risks of Hazards, Personal Protective Equipment (PPE) - Hair, Dressing for the Laboratory, Eye Protection, Eyewash fountain, Gloves, Laboratory Protocols, Labeling Chemicals, Careful reading of labels Prevention of Inhaling Harmful Chemicals, Guide to Chemical Hazards, Chemical Spills etc., Accidents use of fire extinguisher and first aid kit in the laboratory, safety symbols- Preparation of the charts by the students and display of charts in chemistry labs. Calibration of fractional weights, calibration of glass ware - burette, pipette, standard flask, Normality/Molarity and specific gravity of concentrated acids – Preparation of dilute solutions (Numerical problems). Precautions to be taken in the preparation of dilute acids and bases and bases. Preparation of stock solutions of salts with specific examples. Properties of primary standard salt and preparation of standard solution. Good laboratory practices-maintenance of observation book record.

UNIT 2: Preparation of Lab Reagents **15 h (1 hr/week)**

Preparation of indicators and use of indicators in volumetric analysis- acid base titrations, redox titrations, precipitation titrations and complexometric titrations. Role of an indicator in detecting end point (Phenolphthalein, Methyl orange, Methyl-red, Potassium Chromate, Diphenylamine, EBT, Murexide, etc). Preparation of buffers – pH 10 ammonical buffer and acetate buffer solutions. Preparation of commonly used reagents : Ammonium hydroxide solution, Ammonium molybdate reagent, Ammonium hydrogen phosphate solution, Bayer's reagent, Benedict's solution, Bromine water, Dimethyl glyoxime reagent, 2,4-Dinitrophenyl hydrazine reagent, Eriochrome black-T reagent Fehling solution, Ferric chloride solution, Ferrous sulphate solution, Iodine solution, Molisch's reagent, Nessler's reagent, Neutral FeCl_3 , Schiff's reagent, Silver nitrate solution, Sodium carbonate solution , Sodium hydroxide (Caustic soda) solution, Starch solution, Tollen's reagent. (reference work and submission of assignments). Charts preparation depicting course content.

RECOMMENDED BOOKS

1. Vogel's Text Book of Quantitative Chemical Analysis, 5th edition.
2. Vogel's Text Book of macro and semimicro qualitative inorganic analysis. G. Svehla, 5th edition.
3. Chemistry Reagent Manual Prepared by Chemistry Department, SGTB Khalsa College under DBT's Star College Scheme, University of Delhi (Available: online)
4. American Chemical Society Safety in Academic Chemistry Laboratories 8th edition.

[Course objectives (CO)]: To improve the skills of students in the application of theory and practical knowledge. To fill the gap between theory and practicals. To train the students in understanding laboratory safety rules and to improve the skills in preparation of laboratory reagents]

B.Sc. Chemistry II Year
Semester III
Skill Enhancement Course- II (SEC –II) (2 Credits)
REMEDIAL METHODS FOR POLLUTION, DRINKING WATER AND SOIL
FERTILITY STANDARDS

UNIT I: Remedial Methods for Pollution Prevention and control of air pollution
15 h (1 hr/week)

Ozone hole-causes and harm due to ozone depletion. The effect of CFC's in Ozone depletion and their replacements. Global Warming and Greenhouse Effect Precautions to control global warming. Deleterious effect of pollutants - Endangered Monuments- acid rain. Precautions to protect monuments. Sources of Radiation pollution - Chernobyl accident and its Consequences. Radiation effect by the usage of cell phones and protection tips. Deleterious effects of cell phone towers and health hazards.

Sources of water pollution-(i). Pollution due to pesticides and inorganic chemicals, (ii). Thermal pollution (iii). Ground water pollution (iv). Eutrophication.

Methods for control of water pollution and water recycling. Dumping of plastics in rivers & oceans and their effect on aquatic life. Determination of (i) Dissolved Oxygen and (ii) Chemical Oxygen Demand in polluted water - Illustration through charts (or) demonstration of experiments. Sources of soil pollution (i). Plastic bags, (ii). Industrial and (iii). Agricultural sources. Control of soil pollution. Environmental laws in India. Environmental benefits of planting trees.

UNIT II: Drinking Water and Soil Fertility Standards and Analysis
15 h (1 hr/week)

Water Quality and Common Treatments for Private Drinking Water Systems: Drinking Water Standards-Primary Drinking Water Standards : Inorganics, Organics and Volatile Organic Chemicals. Secondary Drinking Water Standards-Inorganics and Physical Problems. Water Testing, Mineral Analysis, Microbiological Tests, Pesticide and Other Organic Chemical Tests. Principle involved in Water Treatment Techniques. (i) Reverse osmosis (ii) Disinfection methods such as chlorination, ultraviolet light, ozonation etc (iii) Chemical oxidation and (iv) Ion exchange (water softeners). Visit to nearby drinking water plants and interaction at sites.

Introduction to Soil Chemistry- Basic Concepts. Effect of pH on nutrient availability. Macronutrients and their effect on plants -Carbon, Hydrogen, Oxygen, Nitrogen and Phosphorus other macronutrients-Calcium, Magnesium and Sulfur. Micronutrients and their effect on plants. Boron ($B_4O_7^{2-}$), Copper (Cu^{2+}), Iron (Fe^{2+} , Fe^{3+}) Manganese (Mn^{2+}) Molybdenum (MoO_4^{2-}) Zinc (Zn^{2+}) Cobalt (Co^{2+}) Chlorine (Cl^-) and Others. Determination of soil nitrogen by Kjeldahl method- Illustration through charts (Or) demonstration of experiment. Visit to nearby agricultural farms and interaction with farmers. Discussion with farmers on the use of Soil Analysis Kits.

References

1. A Text book for 'Remedial methods for pollution, drinking water and soil fertility standards', First Edition, Authors: Dr Mudvath Ravi, Gopu Srinivas, Putta Venkat Reddy, Vuradi Ravi Kumar, Battini Ushaiah, ISBN No. 978-93-5311-183-0.
2. Remedial methods for pollution, drinking water and soil fertility standards, Author: Dr G. Vanjatha.
3. Remedial methods for pollution, drinking water and soil fertility standards, Telugu version, Authors: Dr N. Yogi Babu, Dr. G. Vanajatha, M. Srilatha.
4. Environmental Pollution, download.nos.org/333courseE/10.pdf
5. CFC Replacements, butane.chem.uiuc.edu/pshapley/Environmental/L21/3.html
6. Effects of Acid Rain on Buildings www.air-quality.org.uk/12.php
7. Acid Rain Effects - Buildings - Chemistry
chemistry.elmhurst.edu/vchembook/196buildings.html
8. How to protect national heritage - ways to protect monuments www.youthkiawaaz.com/2011/03/how-to-protect-national-heritage/.
9. Chernobyl nuclear power plant accident - NRC www.nrc.gov/reading-rm/doc-collections/fact-sheets/chernobyl-bg.pdf
10. Side-effects of harmful radiation from mobile phones and towers
pib.nic.in/newsite/printrelease.aspx?relid=116304
11. Cell Phone Radiation Protection - Highly Effective Tips <https://www.electricsense.com/775/how-to-protect-yourself-from-cell-phone-radiation/>
12. Chemical Waste That Impact on Aquatic Life or Water Quality
blog.idrenvironmental.com/chemical-waste-that-impact-on-aquatic-life-or-waterquality
13. Trees and Your Environment - Clean Air Gardening
www.cleanairgardening.com/plantingtrees
14. water quality and common treatments for private drinking water . extension.uga.edu/publications/detail.html?number=b939
15. Soil chemistry <https://casfs.ucsc.edu/about/publications/Teaching-Organic-Farming/PDFdownloads/2.2-soil-chemistry.pdf>
16. Soil Analysis-Determination of Available Nitrogen ... - Amrita Virtual Lab
vlab.amrita.edu/?sub=2&brch=294&sim=1551&cnt=1
17. Determination of dissolved oxygen (DO)
www.cutm.ac.in/pdf/env%20engg%20lab%20manual.pdf
18. Determination of chemical oxygen demand of wastewater www.pharmaguideline.com › quality control › test

B.Sc. Chemistry II Year
Semester - IV
Skill Enhancement Course- III (SEC - III) (2 Credits)
Materials and their Applications

Unit – I: Types of Materials

15 h (1 hr/week)

Introduction: Materials and their importance. Classification of Materials, Advanced materials and their need. Types of Materials: Metals, ceramics, polymers and composites; Nature of bonding (Type of bond present). Types and applications of metal alloys: Classification- ferrous and non-ferrous alloys. Ferrous alloys -types and their applications. Non-ferrous alloys – Cu, Al, Ti alloys, their applications and super alloys.

Field Work- Collection of Metal Alloy Samples.

Types and Applications of Ceramics: Classification of Ceramics based on their application- glasses, clay products, refractories, abrasives, cements, and advanced ceramics. Glasses: Compositions and Characteristics of Some of the Common Commercial Glasses; Properties and applications of glass ceramics - preparation of charts depicting various types of glass and their use. Clay products: Structural clay products and the white wares. Refractories: Compositions of four Common Ceramic Refractory Materials, fireclay, silica, basic refractories ex. MgO and special refractories ex. Alumina and Zirconia Cements: Classification, preparation of cement and the setting process; quick setting cements; applications.

Field Work-Visit to industries and collection of samples of materials

Unit – II: Types of Polymers and Applications

15 h (1 hr/week)

Classification of Polymeric materials based on application: Coatings, adhesives, films, foams with examples Polymer Additives: Fillers, Plasticizers, Stabilizers, Colorants, Flame Retardants with examples.

Advanced Materials: Types of advanced materials - semiconductors, bio-compatible materials, smart materials, advanced polymeric materials and nano-engineered materials. Biocompatible materials: Definition. Materials used as biomaterials and their properties. Metals and alloys used in bone and joint replacement. Filling and restoration materials – dental cements, dental amalgams, dental adhesives.

Field Work- Visit to Dental Clinics and interaction with Doctors regarding materials used in Dental treatments.

Smart materials: Shape memory alloys- definition and examples (Ni-Ti alloys, Cu based alloys), applications. Conducting polymers: - Introduction, Electrically conducting polymers and their uses (polyaniline, polypyrrole, polyacetylene and polythiophene).

References

1. William D. Callister Materials Science and Engineering An Introduction, John Wiley & Sons, Inc, 2006.
2. Material science by Kakani and Kakani.
3. Sujata V., Bhat., —Biomaterials, Narosa Publication House, New Delhi, 2002.
4. M. V. Gandhi and B. S. Thompson, —Smart Materials and Structures, Chapman and Hall, London, First Edition, 1992.
5. Duerig, T. W., Melton, K. N, Stockel, D. and Wayman, C.M., —Engineering aspects of Shapememory Alloys, Butterworth – Heinemann, 1990.
6. Conducting Polymers, Fundamentals and Applications A Practical Approach Authors: Chandrasekhar, Prasanna Ashwin-Ushas Corp., Inc. Kluwer Academic Publishers. Boston

B.Sc. Chemistry II Year Semester IV
Skill Enhancement Course- IV (SEC - IV) (2 Credits)
Chemistry of Cosmetics and Food Processing

Unit-I: Chemistry of Cosmetics and Perfumes

A general study including preparation and uses of the following: Hair dye, hair spray, shampoo, sunscreen lotions, lipsticks, talcum powder, nail enamel, creams (cold, vanishing and shaving creams), antiperspirants and artificial flavours. Essential oils and their importance in cosmetic industries with reference to eugenol, geraniol, sandalwood oil, eucalyptus, 2-phenyl ethyl alcohol. Demonstration experiments or illustration of experimental procedures through charts for the preparation of talcum powder, shampoo and vanishing cream. Analysis of deodorants and antiperspirant - Aluminum, Zinc, Boric acid, Chloride and Sulphide.

Unit-II: Food Processing and Food Adulteration

Food processing: Introduction, methods for food processing, additives and preservatives. Food processing- impact on nutrition, analysis of calcium in milk by complexometric titration, spectrophotometric analysis of iron in foods, Spectrophotometric identification and determination of caffeine and benzoic acid in soft drinks. Field Work -Visit to Food Industries. Food adulteration: Adulterants in some common food items and their identification: Pulses, chilli powder, turmeric powder, milk, honey, spices, food grains and wheat flour, coffee powder, tea leaves, vegetable oil, ghee, ice creams, tomato sauce. Field Work-Collection of adulterated food samples, demonstration of a minimum of five experiments for testing adulterants in food items.

References

1. E. Stocchi: Industrial Chemistry, Vol -I, Ellis Horwood Ltd. UK.
2. P.C. Jain, M. Jain: Engineering Chemistry, Dhanpat Rai & Sons, Delhi
3. Sharma, B.K. & Gaur, H. Industrial Chemistry, Goel Publishing House, Meerut (1996).
4. Rameen Devi, Food Processing and Impact on Nutrition, Sc J Agric Vet Sci., AugSep 2015; 2(4A):304-311.
5. W.A. Poucher, Perfumes, Cosmetics and Soaps (1993).
6. Srilakshmi, Food Science. Edition: 3rd (2004). 7. Lillian Hoagland Meyer, Food chemistry (2008).
8. Handbook of Analysis and Quality Control for Fruit and Vegetable Products, S. Ranganna, Tata McGraw-Hill Education, 1986 – Food.
9. Fundamental concepts of applied chemistry J.C Ghosh, S. Chand and Co, Ltd, New Delhi.
10. Applied Chemistry K .Bhagavathi Sundhar, MJP publishers.

B.Sc., Chemistry, III Year, CBCS Syllabus

Telangana State Council of Higher Education, Govt. of Telangana B.Sc, CBCS Common
Core Syllabi for all Universities in Telangana
PROPOSED SCHEME FOR CHOICE BASED CREDIT SYSTEM IN
B.Sc., Chemistry (for the batch admitted in 2019-2020)

THIRD YEAR- SEMESTER V				
CODE	COURSE TITLE	COURSE TYPE	HPW	CREDITS
BS 501	Chemistry of Cosmetics, Food Processing, Drugs and Pharmaceuticals	GE	4	4
BS 502	English	CC-1E	3	3
BS 503	Second language	CC-2E	3	3
BS 504	Optional- I A/B	DSE -1E	-----	4+1=5
BS 505	Optional- II A/B	DSE -2E	-----	4+1=5
BS 506	Optional- III A/B A. Spectroscopy and Chromatography (or) B. Metallurgy, Dyes and Catalysis	DSE -3E	$\left. \begin{matrix} 4T \\ 3P \end{matrix} \right\} = 7$	$\left. \begin{matrix} 4 \\ 1 \end{matrix} \right\} = 5$
	Laboratory Course -V Experiments in Physical Chemistry-I			
	TOTAL			25
THIRD YEAR- SEMESTER VI				
BS 601	Project in Chemistry/ Advanced Chemistry			4
BS 602	English	CC-1F	3	3
BS 603	Second language	CC-2F	3	3
BS 604	Optional- I A/B	DSE-1F	-----	4+1=5
BS 605	Optional- II A/B	DSE -2F	-----	4+1=5
BS 606	Optional- III A/B A. Medicinal Chemistry (or) B. Agricultural and Fuel Chemistry	DSE -3F	$\left. \begin{matrix} 4T \\ 3P \end{matrix} \right\} = 7$	$\left. \begin{matrix} 4 \\ 1 \end{matrix} \right\} = 5$
	Laboratory Course -VI Experiments in Physical Chemistry-II			
	TOTAL			25
	TOTAL Credits			150

Semester V
Generic Elective (GE) Course - I (4 Credits)
(for B.Sc. Non Chemistry/B.A/B.Com Students)
Chemistry of Cosmetics, Food Processing, Drugs and Pharmaceuticals 60Hrs

Unit-I: Chemistry of Cosmetics and Perfumes **15 Hrs**

A general study including preparation and uses of the following: Hair dye, hair spray, shampoo, sunscreen lotions, lipsticks, talcum powder, nail enamel, creams (cold, vanishing and shaving creams), antiperspirants and artificial flavours. Essential oils and their importance in cosmetic industries with reference to eugenol, geraniol, sandalwood oil, eucalyptus, 2-phenyl ethyl alcohol.

Demonstration experiments or illustration of experimental procedures through charts for the preparation of talcum powder, shampoo and vanishing cream. Chemistry and Applications of deodorants and antiperspirant - Aluminum, Zinc, Boric acid, Chloride and Sulphide.

Unit-II: Food Processing and Food Adulteration **15 Hrs**

Food processing: Introduction, methods for food processing, additives and preservatives. Food processing- impact on nutrition,

Food adulteration: Adulterants in some common food items and their identification: Pulses, chilli powder, turmeric powder, milk, honey, spices, food grains and wheat flour, coffee powder, tea leaves, vegetable oil, ghee, ice creams, tomato sauce.

Food Packaging: Definition and function of packaging-Classification of packaging materials-different types of packaging materials such as glass, wood, metal, paper, wood, plastic etc., - advantages and disadvantages of each packaging material. Packaging materials and systems: corrugated fibre board boxes, shrink bundles and reusable packages. Effect of packaging materials on nutritive values of food.

Food labelling: Introduction, need and importance.

Unit – III: General Characteristics of Drugs **15Hrs**

Introduction: Diseases – causes of diseases, Drug – definition and sources.

ADME of drugs (brief) – Absorption, distribution, drug metabolism (in liver), elimination (brief). Toxicity.

Examples (i) Zintac (Ranitidine, antacid) (ii) Paracetamol (antipyretic) (iii) Benadryl (Cough syrup). Characteristics of an ideal drug.

Nomenclature of Drugs: chemical name – generic name – trade name. Trade names for the given generic names – (i) Aspirin (ii) Amoxycillin (iii) Ciprofloxacin (iv) Paracetamol (v) Mebendazole

Drug formulations: Definition – need for conversion of drug into pharmaceutical (drug formulations) – Additives – diluents, binders, lubricants, antioxidants, flavourants, sweeteners, colourants, coating agents. Classification of Drug formulations: oral, parenterals and topical dosage forms –

advantages and disadvantages.

(i) Oral Dosage forms: Tablets (Aspirin – analgesic; Ciprofloxacin - antibacterial). Capsules (Amoxycillin – antibiotic; Omeprazole-antacid). Syrups (B-complex syrup; Benadryl- Cough syrup).

- (ii) **Parenterals (Injection forms):** Propranolol (antihypertensive), Heparin (anticoagulant)
- (iii) **Topical dosage forms:** Creams and Ointments
- (iv) **Antiallergic:** Aclometasone (Aclovate), Betamethasone valerate(2%) Multiple purposes,
- (v) **Anti-itching:** Doxepin (Zonalon), Antifungal: Miconazole (Dactarin, Neomicol), Ketoconazole, (Nizoral Cream), Fluconazole, Anesthetic- Lidocaine, (Lidocaine ointment) and Antiseptic: Boro Plus Cream, For burns -Iodine ointment

Unit – IV: Classification of Drugs

15Hrs

Classification of drugs based on therapeutic action-Chemotherapeutic agents, Pharmacodynamic agents and drugs acting on metabolic processes.

Brief explanation for the following:

- (i) **Chemotherapeutic agents:** Antimalarials – Chloroquine; Antibiotic – Amoxicillin; Antitubercular drugs – isoniazide; Antiprotozoals – metronidazole.
- (ii) **Pharmacodynamic agents**
 - (a) Drugs acting on CNS: Diazepam (CNS depressant), General anesthetic (thiopental sodium), antipyretic and analgesic (Ibuprofen)
 - (b) Drugs acting on PNS: local anaesthetics (Benzocaine)
 - (c) Drugs acting on cardiovascular system: Metoprolol (antihypertensive agents), Nifedipine (antianginal and antihypertensive agent)
 - (d) Drugs acting on renal system: Diuretics (Acetazolamide)
- (iii) **Drugs acting on metabolic processes**
 - (a) Vitamins: Common name, source, deficiency, vitamin A, B2, B6, C, D, E and K – remedy
 - (b) Hormones: Function (brief) - deficiency of hormones (Insulin, Testosterone and Oestrogen)

Recommended Text Books and Reference Books

1. Industrial Chemistry, Vol -I, E. Stocchi, Ellis Horwood Ltd. UK.
2. Engineering Chemistry, P.C. Jain, M. Jain, Dhanpat Rai & Sons, Delhi.
3. Industrial Chemistry, Sharma, B.K. & Gaur, H. , Goel Publishing House, Meerut (1996).
4. Food Processing and Impact on Nutrition, Rameen Devi, Sc J Agric Vet Sci., Aug-Sep 2015; 2(4A):304-311.
5. Perfumes, Cosmetics and Soaps , W.A. Poucher, (1993).
6. A first course in food analysis by A Y Sathe
7. Food Science by N.Potter, CBS publishers
8. Food chemistry, Lillian Hoagland Meyer, (2008).
9. A Handbook of food packaging by F. A. Paine and H.Y. Paine.
10. Fundamental concepts of applied chemistry J.C Ghosh, S. Chand and Co, Ltd, New Delhi.
11. Applied Chemistry K .Bhagavathi Sundhar, MJP publishers.
12. Drugs by G.L.David Krupadanam, D.Vijaya Prasad, K.Varaprasad Rao, K.L.N.Reddy, C.Sudhakar , Universities Press (India) Limited 2007.
13. An Introduction to Medicinal Chemistry by Graham L. Patrick, Oxford University Press, New York. 1995

B.Sc. Chemistry III Year
Semester-V, Paper-V
Discipline Specific Elective- A (4 Credits)
Spectroscopy and Chromatography

60Hrs

Unit I: Molecular spectroscopy

15Hrs

S5-E-A-I: Introduction to electromagnetic radiation, interaction of electromagnetic radiations with molecules, various types of molecular spectra.

Rotational spectroscopy (Microwave spectroscopy)

Rotational axis, moment of inertia, classification of molecules (based on moment of inertia), rotational energies, selection rules (No derivation), Determination of bond length of rigid diatomic molecules eg. HCl.

Infra red spectroscopy

Energy levels of simple harmonic oscillator, molecular vibration spectrum, selection rules. Determination of force constant (Problems). Qualitative relation of force constant to bond energies. Anharmonic motion of real molecules and energy levels. Modes of vibrations in polyatomic molecules. Characteristic absorption bands of various functional groups. Finger print nature of infrared spectrum.

Electronic spectroscopy

Bonding and antibonding molecular orbitals, electronic energy levels of molecules (σ , π , n), types of electronic transitions: σ - σ^* , n - σ^* , n - π^* , π - π^* with suitable examples. Selection rules, Terminology of chromophore, auxochrome, bathochromic and hypsochromic shifts. Absorption of characteristics of chromophones: diene, enone and aromatic chromophores. Representation of UV-visible spectra. General features of absorption – spectroscopy, transmittance, absorbance, and molar absorptivity. Beer Lambert's law and its limitations.

Unit II: NMR and Mass Spectrometry

15Hrs

S5-E-A-II: Proton Magnetic Resonance Spectroscopy

Principles of nuclear magnetic resonance, equivalent and non-equivalent protons, position of signals. Chemical shift, factors affecting chemical shifts, NMR splitting of signals – spin-spin coupling, representation of proton NMR spectrum – Integrations. ^1H NMR spectrum of – ethyl bromide, acetaldehyde, 1,1,2-tribromo ethane, ethyl acetate and acetophenone.

Mass Spectrometry

Electron Impact Mass: Basic principles, Nitrogen rule, types of ions: Molecular ion and fragment ions. Representation of mass spectrum, types of peaks (molecular ion peak, base peak and isotopic ion peaks). Determination of molecular formula. Mass spectrum of ethyl chloride, ethyl bromide and acetophenone.

Unit III: Separation techniques - I

15Hrs

S5-E-A-III: Solvent Extraction- Principle, Methods of extraction: Batch extraction, continuous extraction and counter current extraction. Application – Determination of Iron(III).

Chromatography: Classification of chromatographic methods, principles of differential migration, adsorption phenomenon, nature of adsorbents, solvent systems.

Thin layer Chromatography (TLC): Advantages, preparation of plates, Solid phase and mobile phase used in TLC, eluotropic series, development of the chromatogram, Detection of the spots, visualizing agents, factors effecting R_f values and applications of TLC.

Paper Chromatography: Principle, choice of paper and solvent systems, development of chromatogram – ascending, descending, radial and two dimensional chromatography, detection of spots, and applications of paper chromatography.

15Hrs

Unit IV: Separation techniques - II

S5-E-A-IV: Column Chromatography- Principle, Types of stationary phases, Column packing – Wet packing technique, Dry packing technique. Selection criteria of mobile phase solvents for eluting polar, non-polar compounds and its applications.

Ion exchange chromatography: Principle, cation and anion exchange resins, its application in separation of ions, de-ionized water.

Gas Chromatography: Principle, theory and instrumentation (Block Diagram), Types of stationary phases and carrier gases (mobile phase), applications of GC.

High performance liquid chromatography: Principle, theory and instrumentation, stationary phases and mobile phases. Applications of HPLC, Analysis of paracetamol.

Recommended Text Books and Reference Books

1. Fundamentals of Molecular Spectroscopy, Banwell & McCash
2. Organic spectroscopy, William Kemp, Palgrave Macmillan; 2nd Revised edition
3. Spectroscopy, B K Sharma Krishna Prakashan Media, 1981
4. Elements of Organic Spectroscopy, Y R Sharma.
5. Applications of Absorption Spectroscopy of Organic Compounds (English, Paperback, Dyer R. John)
6. Organic Chemistry, Morrison and Boyd, Pearson Publications.
7. Introduction to Spectroscopy by Donald Pavia, Gary Lampman and George Kriz. Saunders College Division, 2001
8. Chemistry text book for B.Sc., published by Telugu Academy, Govt. of Telangana.
9. Analytical Chemistry by David Krupadanam, Universities Press (India) Limited.
10. Principles of Instrumental Analysis, D.A. Skoog, F.J. Holler, T.A. Nieman, Engage Learning India Ed.
11. Fundamentals of Analytical Chemistry 6 th Ed., D. A. Skoog, D.M. West, F.J. Holler, Saunders College Publishing, Fort worth (1992).
12. Instrumental Methods of Analysis. 7th Ed. Willard, H.H., Merritt, L.L., Dean, J. & Settle, F.A. Wordsworth Publishing Co. Ltd., Belmont, California, USA, 1988.
13. A Textbook of Quantitative Inorganic Analysis 7th Ed., Vogel, A. I. Prentice Hall.
14. Analytical Chemistry 7 th edition by Gary D. Christian (2004).
15. Separation Methods, M.N Sastry, Himalaya Publication (2004).

B.Sc. Chemistry III Year
Semester-V, Paper- V
Discipline Specific Elective-B (4 Credits)
Metallurgy, Dyes and Catalysis

60 Hrs

Unit I: General Principles of Metallurgy and Production of Non Ferrous Metals **15 Hrs**
S5-E-B-I: Pyrometallurgy: Drying and calcination, roasting, smelting, products of smelting.
Hydrometallurgy: Leaching methods, leaching agents, leaching of metals, oxides and sulphides.
Separation of liquid and solid phases and processing of aqueous solutions
Electrometallurgy: Electrolysis, Refining electrolysis, electrolysis from aqueous solutions, fused-salt electrolysis
Refining processes: Chemical and physical refining processes
Production of selected non-ferrous metals (Copper, Nickel, Zinc): Properties, raw materials, production (flow charts presentations and chemical reactions involved) and uses.

Unit II: Natural and Synthetic Dyes **15Hrs**
S5-E-B-II: Dyes: Definition, Classification of dyes- Natural dyes, synthetic dyes; based on chemical constitution of dyes; Chemical nature of dyes; Applications of dyes.
Structures of natural dyes: Indigo, Tyrian purple, Alizarin, Indigotin.
Structures of Synthetic Dyes: Nitro dyes, Nitrosodyes, Azodyes (Mono azodyes, bisazodyes), diaryl methane dyes, triaryl methane dyes, Xanthene dyes, Phenolphthalein, Fluorocetin, Acridine dyes.
Synthesis of dyes: Mono azodyes, bisazodyes (Congo red), Auromine O, Malachite Green, Crystal Violet, Rhodamine B, Acridine Yellow, Indigotin .
Binding of dyes to fabric. Applications of dyes.

Unit III: Catalysis I **15Hrs**
S5-E-B-III: Homogeneous and heterogeneous catalysis -
Definition of a catalyst and catalysis. Comparison of homogeneous and heterogeneous catalysis with specific examples. General characteristics of catalytic reactions.
Acid-base catalysis- Examples of acid and base catalysed reactions, hydrolysis of esters.
Kinetics of acid catalysed reactions. Specific acid and general acid catalysis, Kinetics of base catalysed reactions. Specific base and general base catalysis. Examples-Aldol condensation and decomposition of nitramide, base catalysed conversion of acetone to di acetone alcohol. Mutarotation of glucose. Effect of pH on reaction rate of acid and base catalysed reactions.
Phase transfer catalysis: Principle of phase transfer catalysis, classification of phase transfer catalysts. Factors influencing the rate of PTC reactions.

Unit IV: Catalysis II **15Hrs**
S5-E-B-IV: Enzyme catalysis- Characteristics of enzyme catalysis, Examples: (i) Invertase in inversion of cane sugar (ii) Maltase in conversion of maltose to glucose (iii) Urease in decomposition of urea (iv) Zymase in conversion of glucose to ethanol (v) working of carbonic anhydrase and (vi) Mechanism of oxidation of ethanol by alcohol dehydrogenase Factors affecting enzyme catalysis. Effect of temperature, pH, concentration and effect of inhibitor on enzyme catalysed reactions, Catalytic efficiency.

Kinetics of enzyme catalysed reactions: Michaelis-Menton Equation. Mechanism of enzyme catalysed reactions. Significance of Michaelis constant (K_m) and maximum velocity (V_{max}), Lineweaver-Burk plot. Types of enzyme inhibitors

Recommended Text Books and Reference Books

1. Industrial Chemistry, B K Sharma
2. Engineering Chemistry, Jain and Jain
3. Industrial Chemistry E. Stocchi, Vol-I, Ellis Horwood Ltd. UK.
4. Handbook of Industrial Chemistry, J. A. Kent: Riegel's, CBS Publishers, New Delhi.
5. Theory of production of non-ferrous metals and alloys Study. Kateřina Skotnicová, Monika Losertová, Miroslav Kursa
6. The Chemistry of Synthetic Dyes, Volume 4, K Venkataraman Elsevier
7. Organic Chemistry Vol-I by I.L. Finar.
8. Organic Chemistry by Jennice, Gorzinski Smith
9. Natural Dyes: Sources, Chemistry, Application and Sustainability Issues by Sujata Saxena and A. S. M. Raja.
10. Physical Chemistry by Atkins and De Paula, 8 th Edn.
11. Physical Chemistry by Puri, Sharma and Pattania, 2017.
12. Kinetics and mechanism of chemical transformations by Rajarajm and Kuriacose, Published by Macmillan India Ltd.
13. Text book of Physical Chemistry, K.L. Kapoor, Macmillan, 1999.
14. Catalysis, J.C. Kuriacose, Macmillan Macmillan Publishers India Limited, 1980.
15. Phase Transfer Catalysis, Fundamentals, Applications and Industrial perspective, C. M. Stark, C. Liotta & M. Halpern, Academic Press
16. Phase Transfer Catalysis, E. V. Dehmlow & S. S. Dehmlow, Verlag Chemie, Weinheim

Semester - V
Laboratory Course
Paper V Experiments in Physical Chemistry-I

45 h (3 h / w)

1. Distribution law

- a) Determination of molecular status and partition coefficient of benzoic acid in Toluene and water.
- b) Determination of distribution coefficient of acetic acid between n-butanol and water.

2. Electrochemistry

- a) Determination of cell constant of a conductivity cell.
- b) Verification of Ostwald's dilution law- Determination of dissociation constant (K_a) of acetic acid by conductivity measurements.

3. Colorimetry

- a) Verification of Beer's law using KMnO_4
- b) Determination of the concentration of the given KMnO_4 solution.

4. Adsorption

- b) Adsorption of acetic acid on animal charcoal - Verification of Freundlich adsorption isotherm.

5. Physical constants

- a) Surface tension and b) viscosity of liquids. (Demonstration Experiment)

Reference books:

- 1. Senior practical physical chemistry. B. D. Khosla, V.C. Garg, Adarsh Gulati Published by R. Chand & Co.
- 2. Practical Physical Chemistry: B. Vishwanathan and P.S. Raghavan. Viva Books
- 3. Practicals in Physical Chemistry by P.S. Sindhu ISBN-10: 1-4039-2916-5 / 1403929165
ISBN-13: 978-1-4039-2916-7 / 9781403929167

**B.Sc. Chemistry III Year
Semester –VI
Optional for Chemistry Stream
Advanced Chemistry**

60Hrs

Unit-I (Inorganic Chemistry)

15 Hrs

S6-O-I-1: Inorganic reaction mechanisms

4h

Labile and inert complexes, Thermodynamic and kinetic stability based on VBT & CFT: ligand substitution reactions $-S_N1$ and S_N2 in Octahedral complexes; substitution reactions of square planar complexes – Trans effect and applications of trans effect. Reactions of tetrahedral complexes - Hydrolysis of silicon halides and phosphorous oxides.

S6-O-I-2: Boranes and Carboranes

2 h

Definition of clusters. Structures of boranes and carboranes- Wade's rules, closo, nido, arachno boranes and carboranes

S6-O-I-3: Symmetry of molecules

5 h

Symmetry operations and symmetry elements in molecules. definition of axis of symmetry types of C_n , plane of symmetry (σ_h , σ_v , σ_d), center of symmetry and improper rotational axis of symmetry (S_n). Explanation with examples.

S6-O-I-4: Non – aqueous solvents

4 h

Classification and characteristics of a solvent. Reactions in liquid ammonia – physical properties, auto-ionisation, examples of ammono acids and ammono bases. Reactions in liquid ammonia – precipitation, neutralization, solvolysis, solvation - solutions of metals in ammonia, complex formation, redox reactions. Reactions in HF – autoionisation, reactions in HF – precipitation, acid – base reactions, protonation.

Unit-II (Organic Chemistry)

15 Hrs

S6-O-O-1: Pericyclic Reactions

5 h

Concerted reactions, Molecular orbitals of ethene, 1,3-butadiene and allyl radical. Symmetry properties, HOMO, LUMO, thermal and photochemical pericyclic reactions. Types of pericyclic reactions – electrocyclic, cycloaddition and sigmatropic reactions – one example each and their explanation by FMO theory.

S6-O-O-2: Synthetic Strategies

5 h

Terminology – Target molecule (TM), Disconnection approach – Retrosynthesis, Synthon, Synthetic equivalent (SE), Functional group interconversion (FGI), Linear, Convergent synthesis. Retrosynthetic analysis of the following molecules: 1) acetophenone 2) cyclohexene and 3) 2-phenylethanol.

S6-O-O-3: Asymmetric synthesis

5 h

Definition and classification of stereoselective reactions: substrate, product stereoselective reactions, enantio and diastereo selective reactions. Stereospecific reaction – definition –example – dehalogenation of 1,2-dibromides induced by iodide ion. Enantioselective reactions – definition – example –Reduction of Ethylacetoacetate by Yeast. Diastereoselective reaction- definition-

example: Acid catalysed dehydration of 1-phenylpropanal and Grignard addition to 2-phenylpropanal. Definition and explanation of enantiomeric excess and diastereomeric excess.

Unit III (Physical Chemistry)

15 Hrs

S6-O-P--1: Polymers

Definition of polymers – natural polymers and synthetic polymers examples classification as plastics, fibers, elastomers.

Thermosetting, thermoplastic polymers. Branched, cross-linked and co-polymers.

Definition of polymerization-addition and condensation polymerization with examples.

Explanation : chain polymerization, step polymerization, co-polymerization and co-ordination polymerization. Kinetics of free radical polymerization. Tacticity, atacticity, stereo specific synthesis- Zeigler- Natta catalyst.

Molecular weight definitions- number average, weight average molecular weight. Determination of molecular weight of polymers using viscosity method, Osmometric method. Problems.

Preparation and industrial applications of polyethylene, poly vinyl chloride (PVC), nylon -66, teflon, polyacrylonitrile and terelene.

Introduction to biodegradability and examples of biodegradable polymers.

Unit IV: (General Chemistry)

15 Hrs

S6-O-G--1:: Electroanalytical methods

Types of Electroanalytical Methods.

I) Interfacial methods – a) Potentiometry: Principle, Electrochemical cell, Electrodes- (i) Indicator and (ii) Reference electrodes – Normal Hydrogen Electrode, Quinhydrone Electrode, Saturated Calomel Electrode. Numerical Problems. Application of Potentiometry – Assay of Sulphanilamide

b) Voltammetry – three electrode assembly; Introduction to types of voltametric techniques, micro electrodes, Over potential and Polarization.

II) Bulk methods – Conductometry, Conductivity Cell, Specific Conductivity, Equivalent Conductivity. Numerical Problems. Applications of conductometry. Estimation of Cl – using AgNO_3 . Determination of Aspirin with KOH.

Recommended Text Books and Reference books

1. Basic Inorganic Chemistry by F.A.Cotton, G.Wilkinson and Paul.L. Gaus 3 rd edn Wiley Publishers (2001).
2. Inorganic Chemistry Principles of structure and reactivity by James E.Huhey, E.A. Keiter and R.L. Keiter 4 th edn. (2006)
3. Inorganic Chemistry by Shriver and Atkins 3 rd edn Oxford Press (1999).
4. Principles of Inorganic Chemistry by Puri, Sharma and Kalia Vishal Publications (1996).
5. Symmetry and Spectroscopy of Molecules, K. Veera Reddy, Second Edition, New Age International (P) Limited Publishers
6. Textbook of Inorganic Chemistry by R Gopalan, Universities Press,(2012)
7. Text book of organic chemistry by Morrison and Boyd, Pearson Publishers (2009)
8. Text book of organic chemistry by Graham Solomons, Wiley(2015)

9. Fundamentals of organic synthesis and retrosynthetic analysis by Ratna Kumar Kar, NCBA,(2014)
10. Organic synthesis by Dr. Jagadamba Singh and Dr. L.D.S. Yadav, Pragati Prakashan, 2010
11. Stereochemistry of organic compounds by D. Nasipuri, New Academic Science Limited, 2012
12. Organic chemistry by Clayden, Greeves, Warren and Wothers, Oxford University Press, 2001
13. Fundamentals of Asymmetric Synthesis by G. L. David Krupadanam, Universities Press(2014)
14. Polymer Chemistry, M G Arora and M Singh
15. Introductory Polymer Chemistry by G S Misra
16. Textbook of Polymer Science, F. W. Billmeyer Jr, John Wiley & sons
17. Polymer Science, V. R. Gowarikar, N. V. Viswanathan & J. Sreedhar, Wiley Eastern
18. Contemporary Polymer Chemistry, H. R. Alcock & F. W. Lambe, Prentice Hall
19. Materials Science and Engineering An Introduction by William D. Callister, Jr. John Wiley & Sons, Inc.
20. Principles of Instrumental Analysis, D.A. Skoog, F.J. Holler, T.A. Nieman, Engage earning India Ed.
21. Fundamentals of Analytical Chemistry 6 th Ed., D. A. Skoog, D.M. West, F.J. Holler, Saunders College Publishing, Fort worth (1992).
22. Physical Chemistry by Atkins and De Paula, 8 th Edn.
23. Physical Chemistry by Puri, Sharma and Pattania, 2017

**B.Sc. Chemistry III Year
Semester-VI, Paper-VI
Discipline Specific Elective-A (4 Credits)
Medicinal Chemistry**

60Hrs

15Hrs

Unit- I: Introduction and Terminology

S6-E-A-I: Diseases: Common diseases, infective diseases—insect borne, air-borne, water-borne and hereditary diseases.

Terminology in Medicinal Chemistry: Drug, Active Pharmaceutical Ingredient (API), Pharmaceuticals, Pharmacology, Pharmacophore, Pharmacodynamics, Pharmacokinetics, metabolites, anti metabolites and therapeutic index.

Drugs: Nomenclature: Chemical name, Generic name and Trade names with examples; Classification: Classification based on structures and therapeutic activity with examples.

ADMET: a) Absorption: Definition, absorption of drugs across the membrane – active and passive absorption, routes of administration of drugs. b) Distribution: definition and effect of plasma protein binding. c) Metabolism: definition, phase I and phase II reactions. d) Elimination: definition and renal elimination. Toxicity.

Unit-II: Enzymes and Receptors

15Hrs

S6-E-A-II: Enzymes: Introduction. Mechanism and factors affecting enzyme action, Specificity of enzyme action (including stereo specificity), Enzyme inhibitors and their importance. Types of inhibition - reversible, irreversible and their subtypes with examples.

Receptors: Introduction, Drug action-receptor theory, Mechanism of drug action, concept of agonists and antagonists with examples. Drug receptor interactions involved in drug receptor complex. binding role of –OH group, –NH₂ group, quaternary ammonium salts and double bond. Structure – activity relationships of drug molecules, explanation with sulfonamides.

Unit- III: Synthesis and Therapeutic Activity of Drugs

15Hrs

S6-E-A-III: Introduction, synthesis and therapeutic activity of

Chemotherapeutics: Sulphanilamide, dapsone, Pencillin-G (semi synthesis), Chloroquin, Isoniazid, Cisplatin and AZT.

Drugs to treat metabolic disorders: Anti diabetic - Tolbutamide; Antiinflammatory – Ibuprofen; Cardiovascular- Glyceryl trinitrate; Antipyretic (paracetamol, aspirin) and Antacid- Omeprazole.

Drugs acting on nervous system: Anesthetics-definition, Classification-local and general. Volatile- Nitrous oxide, chloroform uses and disadvantages. Local anaesthetics – benzocaine.

Unit- IV: Molecular Messengers, Vitamins and Micronutrients

15Hrs

S6-E-A-IV: Molecular Messengers: Introduction to hormones and neurotransmitters, Thyroid hormones, Antithyroid drug-Carbimazol. Adrenaline: Adrenergic drugs- salbutamol, atenelol. Serotonin: SSRIs- fluoxetine. Dopamine: Antiparkinson drug- Levodopa .

Drug analysis: Concept, Drug stability, Chemical reactions that cause drug degradation, Analytical methods of Drug analysis: Spectrophotometric methods, Chromatographic methods, Quality assurance and quality control, Method validation and statistical interpretation of the analytical Method.

Recommended Text Books and Reference books

1. Introduction to Medicinal Chemistry, G.L. Patrick, Oxford University Press, New York. 2013.
2. Medicinal Chemistry, Thomas Nogrady, Oxford Univ. Press, New York. 2005.
3. Foye's Principles of Medicinal Chemistry, David William and Thomas Lemke, Lippincott Williams & Wilkins, 2008.
4. Medicinal Chemistry, Ashutosh Kar, New Age International, 2005.
5. Synthetic Drugs, O.D.Tyagi & M.Yadav, Anmol Publications, 1998.
6. Medicinal Chemistry, Alka L. Gupta, Pragati Prakashan.
7. Drugs, G. L. David Krupadanam, D.Vijaya Prasad, K.Varaprasad Rao, K. L. N. Reddy, C. Sudhakar, Universities Press (India) Ltd. 2012.
8. Blass B. Basic Principles of Drug Discovery and Development. 1st ed. Amsterdam: Academic Press; 2015
9. Cairns D. Essentials of Pharmaceutical Chemistry. 3rd ed. UK: Pharmaceutical Press; 2008
10. Jeffery GH, Bassett J, Mendham J, Denney RC. Vogel's Textbook of Quantitative Chemical Analysis. 5th ed. England, UK: Longman Scientific and Technical; 1989

B.Sc. Chemistry III Year
Semester –VI, Paper-VI
Discipline Specific Elective-B (4 Credits)
Agricultural and Fuel Chemistry

60 Hrs

Unit I: – Pesticides

15Hrs

S6-E-B-I: Introduction, Definition, classification of pesticides based on use (target). Toxicity and chemical structure with examples. Adverse effects of pesticides and its impact on environmental pollution.

Synthesis, manufacture and uses of representative pesticides: Organochlorines (Cypermethrin); Organophosphates (Parathion); Carbamates (Carbaryl); Quinones (Chloranil), Anilides (Alachlor). **Pesticide formulations**: Dusts, Granules, Wettable powders, Emulsions and Aerosols.

Biopesticides : Introduction: Potential pesticidal plants of India, Role of Neem in plant protection-constituents, Azadirachtin and its role in pest control, Structure and mode of action of Pyrethrins (pyrethrin-1) and Pyrethroids (permethrin) and nicotinoids (Imidacloprid).

Unit II: – Fertilizers

15Hrs

S6-E-B-II: Introduction: (need of fertilizers), functions of essential plant nutrients (N, P, K), Classification formula and uses of fertilizers:

Nitrogenous fertilizers: Ammonium nitrate, Urea, Calcium Cyanamide, Calcium Ammonium Nitrate, Sodium Nitrate, Ammonium Chloride and their uses.

Phosphate fertilizers: Normal super phosphate, Triple Super Phosphate, Ammonium Phosphate and their uses.

Potassium fertilizers: Potassium chloride, potassium nitrate, potassium sulphate and uses. Complex fertilizers: Diammonium Phosphate and mixed fertilizers their uses. Manufacture of urea and Super phosphate of lime and their reactions in the soil.

Biofertilizers – Introduction, definition, classification, Rhizobium, Azotobacter, Azospirillum, Azolla, Blue Green Algae, Vermicomposting and uses.

Organic farming: The principal methods, crop rotation, green manures and compost, biological pest control, and mechanical cultivation and uses.

Unit III: Energy Sources and Coal

15Hrs.

S6-E-B-III: Review of energy sources (renewable and non-renewable). Classification of fuels and their calorific value.

Coal: Uses of coal (fuel and nonfuel) in various industries, its composition, carbonization of coal. Coal gas, producer gas and water gas—composition and uses. Fractionation of coal tar, uses of coal tar based chemicals, requisites of a good metallurgical coke, Coal gasification (Hydro gasification and Catalytic gasification), Coal liquefaction and Solvent Refining.

Unit IV: Petroleum and its products, petrochemicals and non petroleum fuels

15Hrs.

S6-E-B-IV:

Petroleum and its products

Petroleum: Origin, Composition of crude petroleum and classification. Properties- flash point and its determination, Knocking and antiknocking compounds; Octane number. and Cetane number. Distillation of crude petroleum, Fractional Distillation - Principle and process, refining, Fractions and uses. Cracking -Thermal and catalytic cracking, Reforming

Petroleum products – Petrol, Diesel, LPG, Kerosene, Tar and their applications.

Petrochemicals: Vinyl acetate, Propylene oxide, Isoprene and their uses.

Lubricants: Classification of lubricants- Solid, semisolid and liquids; Properties (viscosity, flash point, fire point, cloud point, pour point) and their determination. Functions of lubricants. Mechanism of lubrication.

Non-petroleum fuels: Natural Gas-CNG, LNG, Clean Fuels- H_2 gas, ethanol, Fuel from waste - bio-gas, Fuel from biomass –bio-ethanol, biodiesel, Synthetic fuels- syngas based.

Recommended Text Books and Reference books

1. Chemistry of pesticides, N. N. Melnikov, Springer-Verlag- Technology & Engineering (2012).
2. Pesticide Synthesis Handbook, Thomas A. Unger, Elsevier, (2000).
3. Pesticides, R. Cremllyn, John Wiley, 1980.
4. Manures and Fertilisers, K. Kolay, Published by Atlantic (2007).
5. Sharma, B.K. & Gaur, H. Industrial Chemistry, Goel Publishing House, Meerut (1996).
6. A Text Book of Engineering Chemistry Paperback – 2017 by Shashi Chawla
7. Industrial Chemistry, Vol-I, Stocchi, E, Ellis Horwood Ltd. UK (1990).
8. Jain, P.C. and Jain, M. Engineering Chemistry Dhanpat Rai & Sons, Delhi.
9. Engineering Chemistry by Shashi Chawla, Dhanpat Rai & Sons, Delhi.

Semester - VI
Laboratory course
Paper VI Experiments in Physical Chemistry-II

45h (3 h/w)

1. Kinetics

- a) Determination of specific reaction rate of the hydrolysis of methyl acetate catalyzed by hydrogen ion at room temperature.
- b) Determination of rate of decomposition of hydrogen peroxide catalyzed by FeCl_3 .

2. Electrochemistry

A. Potentiometry:

- a) Determination of redox potential of $\text{Fe}^{2+}/\text{Fe}^{3+}$ by potentiometric titration of ferrous ammonium sulphate vs. potassium dichromate.
- b) Precipitation titration of KCl vs. AgNO_3 -Determination of given concentration of silver nitrate.

B. pH metry:

- a) pH metric titration of strong acid (HCl) vs. strong base- Determination of the concentration of the given acid.
- b) pH metric titration of weak acid(acetic acid) with strong base(NaOH).- Determination of acid dissociation constant (K_a) of weak acid.

3. Conductometry:

- a) Determination of overall order: Saponification of ethyl acetate with NaOH by conductance measurements.

Reference books:

1. Senior practical physical chemistry. B. D. Khosla, V.C. Garg, Adarsh Gulati
2. Advanced Practical Physical chemistry: J.B. Yadav
3. Practical Physical Chemistry: B. Vishwanathan and P.S. Raghavan.
4. Practical in Physical Chemistry: P.S. Sindhu

Semester V
Generic Elective (GE) Course - I (4 Credits)
(for B.Sc. Non Chemistry/B.A/B.Com Students)
Chemistry of Cosmetics, Food Processing, Drugs and Pharmaceuticals 60Hrs

Unit-I: Chemistry of Cosmetics and Perfumes **15 Hrs**

A general study including preparation and uses of the following: Hair dye, hair spray, shampoo, sunscreen lotions, lipsticks, talcum powder, nail enamel, creams (cold, vanishing and shaving creams), antiperspirants and artificial flavours. Essential oils and their importance in cosmetic industries with reference to eugenol, geraniol, sandalwood oil, eucalyptus, 2-phenyl ethyl alcohol.

Demonstration experiments or illustration of experimental procedures through charts for the preparation of talcum powder, shampoo and vanishing cream. Chemistry and Applications of deodorants and antiperspirant - Aluminum, Zinc, Boric acid, Chloride and Sulphide.

Unit-II: Food Processing and Food Adulteration **15 Hrs**

Food processing: Introduction, methods for food processing, additives and preservatives. Food processing- impact on nutrition,

Food adulteration: Adulterants in some common food items and their identification: Pulses, chilli powder, turmeric powder, milk, honey, spices, food grains and wheat flour, coffee powder, tea leaves, vegetable oil, ghee, ice creams, tomato sauce.

Food Packaging: Definition and function of packaging-Classification of packaging materials-different types of packaging materials such as glass, wood, metal, paper, wood, plastic etc., - advantages and disadvantages of each packaging material. Packaging materials and systems: corrugated fibre board boxes, shrink bundles and reusable packages. Effect of packaging materials on nutritive values of food.

Food labelling: Introduction, need and importance.

Unit – III: General Characteristics of Drugs **15Hrs**

Introduction: Diseases – causes of diseases, Drug – definition and sources.

ADME of drugs (brief) – Absorption, distribution, drug metabolism (in liver), elimination (brief). Toxicity.

Examples (i) Zintac (Ranitidine, antacid) (ii) Paracetamol (antipyretic) (iii) Benadryl (Cough syrup). Characteristics of an ideal drug.

Nomenclature of Drugs: chemical name – generic name – trade name. Trade names for the given generic names – (i) Aspirin (ii) Amoxycillin (iii) Ciprofloxacin (iv) Paracetamol (v) Mebendazole

Drug formulations: Definition – need for conversion of drug into pharmaceutical (drug formulations) – Additives – diluents, binders, lubricants, antioxidants, flavourants, sweeteners, colourants, coating agents. Classification of Drug formulations: oral, parenterals and topical dosage forms –

advantages and disadvantages.

(i) Oral Dosage forms: Tablets (Aspirin – analgesic; Ciprofloxacin - antibacterial). Capsules (Amoxycillin – antibiotic; Omeprazole-antacid). Syrups (B-complex syrup; Benadryl- Cough syrup).

- (ii) **Parenterals (Injection forms):** Propranolol (antihypertensive), Heparin (anticoagulant)
- (iii) **Topical dosage forms:** Creams and Ointments
- (iv) **Antiallergic:** Aclometasone (Aclovate), Betamethasone valerate(2%) Multiple purposes,
- (v) **Anti-itching:** Doxepin Zonalon), Antifungal: Miconazole (Dactarin, Neomicol), Ketoconazole, (Nizoral Cream), Fluconazole, Anesthetic- Lidocaine, (Lidocaine ointment) and Antiseptic: Boro Plus Cream, For burns -Iodine ointment

Unit – IV: Classification of Drugs

15Hrs

Classification of drugs based on therapeutic action-Chemotherapeutic agents, Pharmacodynamic agents and drugs acting on metabolic processes.

Brief explanation for the following:

(i) **Chemotherapeutic agents:** Antimalarials – Chloroquine; Antibiotic – Amoxicillin; Antitubercular drugs – isoniazide; Antiprotozoals – metronidazole.

(ii) Pharmacodynamic agents

(a) Drugs acting on CNS: Diazepam (CNS depressant), General anesthetic (thiopental sodium), antipyretic and analgesic (Ibuprofen)

(b) Drugs acting on PNS: local anaesthetics (Benzocaine)

(c) Drugs acting on cardiovascular system: Metoprolol (antihypertensive agents), Nifedipine (antihypertensive agent)

(d) Drugs acting on renal system: Diuretics (Acetazolamide)

(iii) Drugs acting on metabolic processes

(a) Vitamins: Common name, source, deficiency, vitamin A, B2, B6, C, D, E and K – remedy

(b) Hormones: Function (brief) - deficiency of hormones (Insulin, Testosterone and Oestrogen)

Recommended Text Books and Reference Books

1. Industrial Chemistry, Vol -I, E. Stocchi, Ellis Horwood Ltd. UK.
2. Engineering Chemistry, P.C. Jain, M. Jain, Dhanpat Rai & Sons, Delhi.
3. Industrial Chemistry, Sharma, B.K. & Gaur, H. , Goel Publishing House, Meerut (1996).
4. Food Processing and Impact on Nutrition, Rameen Devi, Sc J Agric Vet Sci., Aug-Sep 2015; 2(4A):304-311.
5. Perfumes, Cosmetics and Soaps , W.A. Poucher, (1993).
6. A first course in food analysis by A Y Sathe
7. Food Science by N.Potter, CBS publishers
8. Food chemistry, Lillian Hoagland Meyer, (2008).
9. A Handbook of food packaging by F. A. Paine and H.Y. Paine.
10. Fundamental concepts of applied chemistry J.C Ghosh, S. Chand and Co, Ltd, New Delhi.
11. Applied Chemistry K .Bhagavathi Sundhar, MJP publishers.
12. Drugs by G.L.David Krupadanam, D.Vijaya Prasad, K.Varaprasad Rao, K.L.N.Reddy, C.Sudhakar , Universities Press (India) Limited 2007.
13. An Introduction to Medicinal Chemistry by Graham L. Patrick, Oxford University Press, New York. 1995

B.Sc. Chemistry III Year
Semester-V, Paper-V
Discipline Specific Elective- A (4 Credits)
Spectroscopy and Chromatography

60Hrs

Unit I: Molecular spectroscopy

15Hrs

S5-E-A-I: Introduction to electromagnetic radiation, interaction of electromagnetic radiations with molecules, various types of molecular spectra.

Rotational spectroscopy (Microwave spectroscopy)

Rotational axis, moment of inertia, classification of molecules (based on moment of inertia), rotational energies, selection rules (No derivation), Determination of bond length of rigid diatomic molecules eg. HCl.

Infra red spectroscopy

Energy levels of simple harmonic oscillator, molecular vibration spectrum, selection rules. Determination of force constant (Problems). Qualitative relation of force constant to bond energies. Anharmonic motion of real molecules and energy levels. Modes of vibrations in polyatomic molecules. Characteristic absorption bands of various functional groups. Finger print nature of infrared spectrum.

Electronic spectroscopy

Bonding and antibonding molecular orbitals, electronic energy levels of molecules (σ , π , n), types of electronic transitions: $\sigma\text{-}\sigma^*$, $n\text{-}\sigma^*$, $n\text{-}\pi^*$, $\pi\text{-}\pi^*$ with suitable examples. Selection rules, Terminology of chromophore, auxochrome, bathochromic and hypsochromic shifts. Absorption of characteristics of chromophones: diene, enone and aromatic chromophores. Representation of UV-visible spectra. General features of absorption – spectroscopy, transmittance, absorbance, and molar absorptivity. Beer Lambert's law and its limitations.

Unit II: NMR and Mass Spectrometry

15Hrs

S5-E-A-II: Proton Magnetic Resonance Spectroscopy

Principles of nuclear magnetic resonance, equivalent and non-equivalent protons, position of signals. Chemical shift, factors affecting chemical shifts, NMR splitting of signals – spin-spin coupling, representation of proton NMR spectrum – Integrations. ^1H NMR spectrum of – ethyl bromide, acetaldehyde, 1,1,2-tribromo ethane, ethyl acetate and acetophenone.

Mass Spectrometry

Electron Impact Mass: Basic principles, Nitrogen rule, types of ions: Molecular ion and fragment ions. Representation of mass spectrum, types of peaks (molecular ion peak, base peak and isotopic ion peaks). Determination of molecular formula. Mass spectrum of ethyl chloride, ethyl bromide and acetophenone.

Unit III: Separation techniques - I

15Hrs

S5-E-A-III: Solvent Extraction- Principle, Methods of extraction: Batch extraction, continuous extraction and counter current extraction. Application – Determination of Iron(III).

Chromatography: Classification of chromatographic methods, principles of differential migration, adsorption phenomenon, nature of adsorbents, solvent systems.

Thin layer Chromatography (TLC): Advantages, preparation of plates, Solid phase and mobile phase used in TLC, eluotropic series, development of the chromatogram, Detection of the spots, visualizing agents, factors effecting R_f values and applications of TLC.

Paper Chromatography: Principle, choice of paper and solvent systems, development of chromatogram – ascending, descending, radial and two dimensional chromatography, detection of spots, and applications of paper chromatography.

15Hrs

Unit IV: Separation techniques - II

S5-E-A-IV: Column Chromatography- Principle, Types of stationary phases, Column packing – Wet packing technique, Dry packing technique. Selection criteria of mobile phase solvents for eluting polar, non-polar compounds and its applications.

Ion exchange chromatography: Principle, cation and anion exchange resins, its application in separation of ions, de-ionized water.

Gas Chromatography: Principle, theory and instrumentation (Block Diagram), Types of stationary phases and carrier gases (mobile phase), applications of GC.

High performance liquid chromatography: Principle, theory and instrumentation, stationary phases and mobile phases. Applications of HPLC, Analysis of paracetamol.

Recommended Text Books and Reference Books

1. Fundamentals of Molecular Spectroscopy, Banwell & McCash
2. Organic spectroscopy, William Kemp, Palgrave Macmillan; 2nd Revised edition
3. Spectroscopy, B K Sharma Krishna Prakashan Media, 1981
4. Elements of Organic Spectroscopy, Y R Sharma.
5. Applications of Absorption Spectroscopy of Organic Compounds (English, Paperback, Dyer R. John)
6. Organic Chemistry, Morrison and Boyd, Pearson Publications.
7. Introduction to Spectroscopy by Donald Pavia, Gary Lampman and George Kriz. Saunders College Division, 2001
8. Chemistry text book for B.Sc., published by Telugu Academy, Govt. of Telangana.
9. Analytical Chemistry by David Krupadanam, Universities Press (India) Limited.
10. Principles of Instrumental Analysis, D.A. Skoog, F.J. Holler, T.A. Nieman, Engage earning India Ed.
11. Fundamentals of Analytical Chemistry 6 th Ed., D. A. Skoog, D.M. West, F.J. Holler, Saunders College Publishing, Fort worth (1992).
12. Instrumental Methods of Analysis. 7th Ed. Willard, H.H., Merritt, L.L., Dean, J. & Settle, F.A. Wordsworth Publishing Co. Ltd., Belmont, California, USA, 1988.
13. A Textbook of Quantitative Inorganic Analysis 7th Ed., Vogel, A. I. Prentice Hall.
14. Analytical Chemistry 7 th edition by Gary D. Christian (2004).
15. Separation Methods, M.N Sastry, Himalaya Publication (2004).

B.Sc. Chemistry III Year
Semester-V, Paper- V
Discipline Specific Elective-B (4 Credits)
Metallurgy, Dyes and Catalysis

60 Hrs

Unit I: General Principles of Metallurgy and Production of Non Ferrous Metals 15 Hrs

S5-E-B-I: Pyrometallurgy: Drying and calcination, roasting, smelting, products of smelting.

Hydrometallurgy: Leaching methods, leaching agents, leaching of metals, oxides and sulphides.

Separation of liquid and solid phases and processing of aqueous solutions

Electrometallurgy: Electrolysis, Refining electrolysis, electrolysis from aqueous solutions, fused-salt electrolysis

Refining processes: Chemical and physical refining processes

Production of selected non-ferrous metals (Copper, Nickel, Zinc): Properties, raw materials, production (flow charts presentations and chemical reactions involved) and uses.

Unit II: Natural and Synthetic Dyes 15Hrs

S5-E-B-II: Dyes: Definition, Classification of dyes- Natural dyes, synthetic dyes; based on chemical constitution of dyes; Chemical nature of dyes; Applications of dyes.

Structures of natural dyes: Indigo, Tyrian purple, Alizarin, Indigotin.

Structures of Synthetic Dyes: Nitro dyes, Nitroso dyes, Azodyes (Mono azodyes, bisazodyes), diaryl methane dyes, triaryl methane dyes, Xanthene dyes, Phenolphthalein, Fluorocin, Acridine dyes.

Synthesis of dyes: Mono azodyes, bisazodyes (Congo red), Auromine O, Malachite Green, Crystal Violet, Rhodamine B, Acridine Yellow, Indigotin .

Binding of dyes to fabric. Applications of dyes.

Unit III: Catalysis I 15Hrs

S5-E-B-III: Homogeneous and heterogeneous catalysis -

Definition of a catalyst and catalysis. Comparison of homogeneous and heterogeneous catalysis with specific examples. General characteristics of catalytic reactions.

Acid-base catalysis- Examples of acid and base catalysed reactions, hydrolysis of esters.

Kinetics of acid catalysed reactions. Specific acid and general acid catalysis, Kinetics of base catalysed reactions. Specific base and general base catalysis. Examples-Aldol condensation and decomposition of nitramide, base catalysed conversion of acetone to di acetone alcohol. Mutarotation of glucose. Effect of pH on reaction rate of acid and base catalysed reactions.

Phase transfer catalysis: Principle of phase transfer catalysis, classification of phase transfer catalysts. Factors influencing the rate of PTC reactions.

Unit IV: Catalysis II 15Hrs

S5-E-B-IV: Enzyme catalysis- Characteristics of enzyme catalysis, Examples: (i) Invertase in inversion of cane sugar (ii) Maltase in conversion of maltose to glucose (iii) Urease in decomposition of urea (iv) Zymase in conversion of glucose to ethanol (v) working of carbonic anhydrase and (vi) Mechanism of oxidation of ethanol by alcohol dehydrogenase Factors affecting enzyme catalysis. Effect of temperature, pH, concentration and effect of inhibitor on enzyme catalysed reactions, Catalytic efficiency.

Kinetics of enzyme catalysed reactions: Michaelis-Menton Equation. Mechanism of enzyme catalysed reactions. Significance of Michaelis constant (K_m) and maximum velocity (V_{max}), Lineweaver-Burk plot. Types of enzyme inhibitors

Recommended Text Books and Reference Books

1. Industrial Chemistry, B K Sharma
2. Engineering Chemistry, Jain and Jain
3. Industrial Chemistry E. Stocchi, Vol-I, Ellis Horwood Ltd. UK.
4. Handbook of Industrial Chemistry, J. A. Kent: Riegel's, CBS Publishers, New Delhi.
5. Theory of production of non-ferrous metals and alloys Study. Kateřina Skotnicová, Monika Losertová, Miroslav Kursa
6. The Chemistry of Synthetic Dyes, Volume 4, K Venkataraman Elsevier
7. Organic Chemistry Vol-I by I.L. Finar.
8. Organic Chemistry by Jennice, Gorzinski Smith
9. Natural Dyes: Sources, Chemistry, Application and Sustainability Issues by Sujata Saxena and A. S. M. Raja.
10. Physical Chemistry by Atkins and De Paula, 8 th Edn.
11. Physical Chemistry by Puri, Sharma and Pattania, 2017.
12. Kinetics and mechanism of chemical transformations by Rajarajm and Kuraiacose, Published by Macmillan India Ltd.
13. Text book of Physical Chemistry, K.L. Kapoor, Macmillan, 1999.
14. Catalysis, J.C. Kuriacose, Macmillan Macmillan Publishers India Limited, 1980.
15. Phase Transfer Catalysis, Fundamentals, Applications and Industrial perspective, C. M. Stark, C. Liotta & M. Halpern, Academic Press
16. Phase Transfer Catalysis, E. V. Dehmlow & S. S. Dehmlow, Verlag Chemie, Weinheim

Semester - V
Laboratory Course
Paper V Experiments in Physical Chemistry-I

45 h (3 h / w)

1. Distribution law

- a) Determination of molecular status and partition coefficient of benzoic acid in Toluene and water.
- b) Determination of distribution coefficient of acetic acid between n-butanol and water.

2. Electrochemistry

- a) Determination of cell constant of a conductivity cell.
- b) Verification of Ostwald's dilution law- Determination of dissociation constant (K_a) of acetic acid by conductivity measurements.

3. Colorimetry

- a) Verification of Beer's law using KMnO_4
- b) Determination of the concentration of the given KMnO_4 solution.

4. Adsorption

- b) Adsorption of acetic acid on animal charcoal - Verification of Freundlich adsorption isotherm.

5. Physical constants

- a) Surface tension and b) viscosity of liquids. (Demonstration Experiment)

Reference books:

- 1. Senior practical physical chemistry. B. D. Khosla, V.C. Garg, Adarsh Gulati Published by R. Chand & Co.
- 2. Practical Physical Chemistry: B. Vishwanathan and P.S. Raghavan. Viva Books
- 3. Practicals in Physical Chemistry by P.S. Sindhu ISBN-10: 1-4039-2916-5 / 1403929165
ISBN-13: 978-1-4039-2916-7 / 9781403929167

B.Sc. Chemistry III Year
Semester –VI
Optional for Chemistry Stream
Advanced Chemistry

60Hrs

Unit-I (Inorganic Chemistry)

15 Hrs

S6-O-I-1: Inorganic reaction mechanisms

4h

Labile and inert complexes, Thermodynamic and kinetic stability based on VBT & CFT: ligand substitution reactions – S_N1 and S_N2 in Octahedral complexes; substitution reactions of square planar complexes – Trans effect and applications of trans effect. Reactions of tetrahedral complexes - Hydrolysis of silicon halides and phosphorous oxides.

S6-O-I-2: Boranes and Carboranes

2 h

Definition of clusters. Structures of boranes and carboranes- Wade's rules, closo, nido, arachno boranes and carboranes

S6-O-I-3: Symmetry of molecules

5 h

Symmetry operations and symmetry elements in molecules. definition of axis of symmetry types of C_n , plane of symmetry (σ_h , σ_v , σ_d), center of symmetry and improper rotational axis of symmetry (S_n). Explanation with examples.

S6-O-I-4: Non – aqueous solvents

4 h

Classification and characteristics of a solvent. Reactions in liquid ammonia – physical properties, auto-ionisation, examples of ammono acids and ammono bases. Reactions in liquid ammonia – precipitation, neutralization, solvolysis, solvation - solutions of metals in ammonia, complex formation, redox reactions. Reactions in HF – autoionisation, reactions in HF – precipitation, acid – base reactions, protonation.

Unit-II (Organic Chemistry)

15 Hrs

S6-O-O-1: Pericyclic Reactions

5 h

Concerted reactions, Molecular orbitals of ethene, 1,3-butadiene and allyl radical. Symmetry properties, HOMO, LUMO, thermal and photochemical pericyclic reactions. Types of pericyclic reactions – electrocyclic, cycloaddition and sigmatropic reactions – one example each and their explanation by FMO theory.

S6-O-O-2: Synthetic Strategies

5 h

Terminology – Target molecule (TM), Disconnection approach – Retrosynthesis, Synthon, Synthetic equivalent (SE), Functional group interconversion (FGI), Linear, Convergent synthesis. Retrosynthetic analysis of the following molecules: 1) acetophenone 2) cyclohexene and 3) 2-phenylethanol.

S6-O-O-3: Asymmetric synthesis

5 h

Definition and classification of stereoselective reactions: substrate, product stereoselective reactions, enantio and diastereo selective reactions. Stereospecific reaction – definition –example – dehalogenation of 1,2-dibromides induced by iodide ion. Enantioselective reactions – definition – example –Reduction of Ethylacetoacetate by Yeast. Diastereoselective reaction- definition-

example: Acid catalysed dehydration of 1-phenylpropanal and Grignard addition to 2-phenylpropanal. Definition and explanation of enantiomeric excess and diastereomeric excess.

Unit III (Physical Chemistry)

15 Hrs

S6-O-P--1: Polymers

Definition of polymers – natural polymers and synthetic polymers examples classification as plastics, fibers, elastomers.

Thermosetting, thermoplastic polymers. Branched, cross-linked and co-polymers.

Definition of polymerization-addition and condensation polymerization with examples.

Explanation : chain polymerization, step polymerization, co-polymerization and co-ordination polymerization. Kinetics of free radical polymerization. Tacticity, atacticity, stereo specific synthesis- Zeigler- Natta catalyst.

Molecular weight definitions- number average, weight average molecular weight. Determination of molecular weight of polymers using viscosity method, Osmometric method. Problems.

Preparation and industrial applications of polyethylene, poly vinyl chloride (PVC), nylon –66, teflon, polyacrylonitrile and terelene.

Introduction to biodegradability and examples of biodegradable polymers.

Unit IV: (General Chemistry)

15 Hrs

S6-O-G--1:: Electroanalytical methods

Types of Electroanalytical Methods.

I) Interfacial methods – a) Potentiometry: Principle, Electrochemical cell, Electrodes- (i) Indicator and (ii) Reference electrodes – Normal Hydrogen Electrode, Quinhydrone Electrode, Saturated Calomel Electrode. Numerical Problems. Application of Potentiometry – Assay of Sulphanilamide
b) Voltammetry – three electrode assembly; Introduction to types of voltametric techniques, micro electrodes, Over potential and Polarization.

II) Bulk methods – Conductometry, Conductivity Cell, Specific Conductivity, Equivalent Conductivity. Numerical Problems. Applications of conductometry. Estimation of Cl – using AgNO_3 . Determination of Aspirin with KOH.

Recommended Text Books and Reference books

1. Basic Inorganic Chemistry by F.A.Cotton, G.Wilkinson and Paul.L. Gaus 3 rd edn Wiley Publishers (2001).
2. Inorganic Chemistry Principles of structure and reactivity by James E.Huhey, E.A. Keiter and R.L. Keiter 4 th edn. (2006)
3. Inorganic Chemistry by Shriver and Atkins 3 rd edn Oxford Press (1999).
4. Principles of Inorganic Chemistry by Puri, Sharma and Kalia Vishal Publications (1996).
5. Symmetry and Spectroscopy of Molecules, K. Veera Reddy, Second Edition, New Age International (P) Limited Publishers
6. Textbook of Inorganic Chemistry by R Gopalan, Universities Press,(2012)
7. Text book of organic chemistry by Morrison and Boyd, Pearson Publishers (2009)
8. Text book of organic chemistry by Graham Solomons, Wiley(2015)

9. Fundamentals of organic synthesis and retrosynthetic analysis by Ratna Kumar Kar, NCBA,(2014)
10. Organic synthesis by Dr. Jagadamba Singh and Dr. L.D.S. Yadav, Pragati Prakashan, 2010
11. Stereochemistry of organic compounds by D. Nasipuri, New Academic Science Limited, 2012
12. Organic chemistry by Clayden, Greeves, Warren and Wothers, Oxford University Press, 2001
13. Fundamentals of Asymmetric Synthesis by G. L. David Krupadanam, Universities Press(2014)
14. Polymer Chemistry, M G Arora and M Singh
15. Introductory Polymer Chemistry by G S Misra
16. Textbook of Polymer Science, F. W. Billmeyer Jr, John Wiley & sons
17. Polymer Science, V. R. Gowarikar, N. V. Viswanathan & J. Sreedhar, Wiley Eastern
18. Contemporary Polymer Chemistry, H. R. Alcock & F. W. Lambe, Prentice Hall
19. Materials Science and Engineering An Introduction by William D. Callister, Jr. John Wiley & Sons, Inc.
20. Principles of Instrumental Analysis, D.A. Skoog, F.J. Holler, T.A. Nieman, Engage earning India Ed.
21. Fundamentals of Analytical Chemistry 6 th Ed., D. A. Skoog, D.M. West, F.J. Holler, Saunders College Publishing, Fort worth (1992).
22. Physical Chemistry by Atkins and De Paula, 8 th Edn.
23. Physical Chemistry by Puri, Sharma and Pattania, 2017

B.Sc. Chemistry III Year
Semester-VI, Paper-VI
Discipline Specific Elective-A (4 Credits)
Medicinal Chemistry

60Hrs

15Hrs

Unit- I: Introduction and Terminology

S6-E-A-I: Diseases: Common diseases, infective diseases—insect borne, air-borne, water-borne and hereditary diseases.

Terminology in Medicinal Chemistry: Drug, Active Pharmaceutical Ingredient (API), Pharmaceuticals, Pharmacology, Pharmacophore, Pharmacodynamics, Pharmacokinetics, metabolites, anti metabolites and therapeutic index.

Drugs: Nomenclature: Chemical name, Generic name and Trade names with examples; Classification: Classification based on structures and therapeutic activity with examples.

ADMET: a) Absorption: Definition, absorption of drugs across the membrane – active and passive absorption, routes of administration of drugs. b) Distribution: definition and effect of plasma protein binding. c) Metabolism: definition, phase I and phase II reactions. d) Elimination: definition and renal elimination. Toxicity.

Unit-II: Enzymes and Receptors

15Hrs

S6-E-A-II: Enzymes: Introduction. Mechanism and factors affecting enzyme action, Specificity of enzyme action (including stereo specificity), Enzyme inhibitors and their importance. Types of inhibition - reversible, irreversible and their subtypes with examples.

Receptors: Introduction, Drug action-receptor theory, Mechanism of drug action, concept of agonists and antagonists with examples. Drug receptor interactions involved in drug receptor complex. binding role of –OH group, –NH₂ group, quaternary ammonium salts and double bond. Structure – activity relationships of drug molecules, explanation with sulfonamides.

Unit- III: Synthesis and Therapeutic Activity of Drugs

15Hrs

S6-E-A-III: Introduction, synthesis and therapeutic activity of

Chemotherapeutics: Sulphanilamide, dapsone, Pencillin-G (semi synthesis), Chloroquin, Isoniazid, Cisplatin and AZT.

Drugs to treat metabolic disorders: Anti diabetic - Tolbutamide; Antiinflammatory – Ibuprofen; Cardiovascular- Glyceryl trinitrate; Antipyretic (paracetamol, aspirin) and Antacid- Omeprazole.

Drugs acting on nervous system: Anesthetics-definition, Classification-local and general. Volatile- Nitrous oxide, chloroform uses and disadvantages. Local anaesthetics – benzocaine.

Unit- IV: Molecular Messengers, Vitamins and Micronutrients

15Hrs

S6-E-A-IV: Molecular Messengers: Introduction to hormones and neurotransmitters, Thyroid hormones, Antithyroid drug-Carbimazol. Adrenaline: Adrenergic drugs- salbutamol, atenolol. Serotonin: SSRIs- fluoxetine. Dopamine: Antiparkinson drug- Levodopa .

Vitamins and Micronutrients: Introduction, vitamin sources, Deficiency disorders and remedy of Vitamins A,B, C, D, E K and micronutrients – Na, K, Ca, Cu, Zn and I .

Recommended Text Books and Reference books

1. Introduction to Medicinal Chemistry, G.L. Patrick, Oxford University Press, New York. 2013.
2. Medicinal Chemistry, Thomas Nogrady, Oxford Univ. Press, New York.2005.
3. Foye's Principles of Medicinal Chemistry, David William and Thomas Lemke, Lippincott Williams & Wilkins, 2008.
4. Medicinal Chemistry, Ashutosh Kar , New Age International, 2005.
5. Synthetic Drugs, O.D.Tyagi & M.Yadav, Anmol Publications,1998.
6. Medicinal Chemistry, Alka L. Gupta, Pragati Prakashan.
7. Drugs, G. L. David Krupadanam, D.Vijaya Prasad, K.Varaprasad Rao, K. L. N. Reddy, C. Sudhakar, Universities Press (India) Ltd. 2012.

B.Sc. Chemistry III Year
Semester –VI, Paper-VI
Discipline Specific Elective-B (4 Credits)
Agricultural and Fuel Chemistry

60 Hrs

Unit I: – Pesticides

15Hrs

S6-E-B-I: Introduction, Definition, classification of pesticides based on use (target). Toxicity and chemical structure with examples. Adverse effects of pesticides and its impact on environmental pollution.

Synthesis, manufacture and uses of representative pesticides: Organochlorines (Cypermethrin); Organophosphates (Parathion); Carbamates (Carbaryl); Quinones (Chloranil), Anilides (Alachlor).

Pesticide formulations: Dusts, Granules, Wettable powders, Emulsions and Aerosols.

Biopesticides : Introduction: Potential pesticidal plants of India, Role of Neem in plant protection-constituents, Azadirachtin and its role in pest control, Structure and mode of action of Pyrethrins (pyrethrin-1) and Pyrethroids (permethrin) and nicotinoids (Imidacloprid).

Unit II: – Fertilizers

15Hrs

S6-E-B-II: Introduction: (need of fertilizers), functions of essential plant nutrients (N, P, K), Classification formula and uses of fertilizers:

Nitrogenous fertilizers: Ammonium nitrate, Urea, Calcium Cyanamide, Calcium Ammonium Nitrate, Sodium Nitrate, Ammonium Chloride and their uses.

Phosphate fertilizers: Normal super phosphate, Triple Super Phosphate, Ammonium Phosphate and their uses.

Potassium fertilizers: Potassium chloride, potassium nitrate, potassium sulphate and uses. Complex fertilizers: Diammonium Phosphate and mixed fertilizers their uses. Manufacture of urea and Super phosphate of lime and their reactions in the soil.

Biofertilizers – Introduction, definition, classification, Rhizobium, Azatobactor, Azospirillum, Azolla, Blue Green Algae, Vermicomposting and uses.

Organic farming: The principal methods, crop rotation, green manures and compost, biological pest control, and mechanical cultivation and uses.

Unit III: Energy Sources and Coal

15Hrs.

S6-E-B-III: Review of energy sources (renewable and non-renewable). Classification of fuels and their calorific value.

Coal: Uses of coal (fuel and nonfuel) in various industries, its composition, carbonization of coal. Coal gas, producer gas and water gas—composition and uses. Fractionation of coal tar, uses of coal tar based chemicals, requisites of a good metallurgical coke, Coal gasification (Hydro gasification and Catalytic gasification), Coal liquefaction and Solvent Refining.

Unit IV: Petroleum and its products, petrochemicals and non petroleum fuels

15Hrs.

S6-E-B-IV:

Petroleum and its products

Petroleum: Origin, Composition of crude petroleum and classification. Properties- flash point and its determination, Knocking and antiknocking compounds; Octane number. and Cetane number. Distillation of crude petroleum, Fractional Distillation - Principle and process, refining, Fractions and uses. Cracking -Thermal and catalytic cracking, Reforming

Petroleum products – Petrol, Diesel, LPG, Kerosene, Tar and their applications.

Petrochemicals: Vinyl acetate, Propylene oxide, Isoprene and their uses.

Lubricants: Classification of lubricants- Solid, semisolid and liquids; Properties (viscosity, flash point, fire point, cloud point, pour point) and their determination. Functions of lubricants. Mechanism of lubrication.

Non-petroleum fuels: Natural Gas-CNG, LNG, Clean Fuels- H_2 gas, ethanol, Fuel from waste - bio-gas, Fuel from biomass –bio-ethanol, biodiesel, Synthetic fuels- syngas based.

Recommended Text Books and Reference books

1. Chemistry of pesticides, N. N. Melnikov, Springer-Verlag- Technology & Engineering (2012).
2. Pesticide Synthesis Handbook, Thomas A. Unger, Elsevier, (2000).
3. Pesticides, R. Cremlyn, John Wiley, 1980.
4. Manures and Fertilisers, K. Kolay, Published by Atlantic (2007).
5. Sharma, B.K. & Gaur, H. Industrial Chemistry, Goel Publishing House, Meerut (1996).
6. A Text Book of Engineering Chemistry Paperback – 2017 by Shashi Chawla
7. Industrial Chemistry, Vol-I, Stocchi, E, Ellis Horwood Ltd. UK (1990).
8. Jain, P.C. and Jain, M. Engineering Chemistry Dhanpat Rai & Sons, Delhi.
9. Engineering Chemistry by Shashi Chawla, Dhanpat Rai & Sons, Delhi.

CERTIFICATE COURSE

In

“Concepts and Analytical techniques in Pharmaceutical chemistry and Organic Synthesis”

Theory (30h)

Unit-I: Chromatography

10h

Chromatography: Classification of chromatographic methods, principles of differential migration, adsorption phenomenon, nature of adsorbents, solvent systems.

Thin layer Chromatography (TLC): Advantages, preparation of plates, development of the chromatogram, Detection of the spots using UV cabinet, factors effecting R_f values and applications.

Column Chromatography- Principle, Types of stationary phases, Column packing – Wet packing technique, Dry packing technique. Selection criteria of mobile phase solvents for eluting polar, non-polar compounds and its applications.

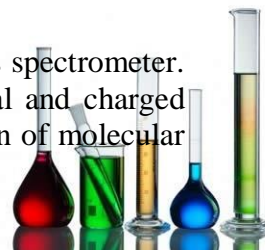
High performance liquid chromatography: Theory and instrumentation, stationary phases and mobile phases. Methods of analysis of purity of compounds.

Unit -II: Spectroscopy-I:

10h

a) **^1H NMR spectroscopy:** Magnetic properties of nuclei, Principles of NMR, equivalent and non equivalent protons, Chemical shifts, factors affecting the chemical shifts, electro negativity and anisotropy, shielding and deshielding effects, Signal integration, Spin-spin coupling: vicinal, germinal and long range, Coupling constants and factors affecting coupling constants. Applications of ^1H NMR spectroscopy: Reaction mechanisms (cyclic bromonium ion, electrophilic and nucleophilic substitutions, carbocations and carbanions), E, Z isomers, conformation of cyclohexane and decalins, keto-enol tautomerism, hydrogen bonding, proton exchange processes (alcohols, amines and carboxylic acids), C-N rotation.

b) **Mass spectrometry:** Origin of mass spectrum, principles of EI mass spectrometer. Types of fragments: odd electron and even electron containing neutral and charged species (even electron rule), Nitrogen rule, isotopic peaks, determination of molecular



formula, metastable ion peaks. High resolution mass spectrometry. Salient features of fragmentation pattern of organic compounds including β -cleavage, McLafferty rearrangement, retro Diels – Alder fragmentation and ortho effect. Principle of EI, CI, Fast Atom Bombardment (FAB), Secondary Ion Mass Spectrometry (SIMS), Electrospray (ESI) ionization and Matrix Assisted Laser Desorption Ionization (MALDI) methods. Introduction to principle and applications of Gas Chromatography-Mass Spectrometry (GC-MS) and Liquid chromatography-Mass Spectrometry (LC-MS) techniques.

Unit -III: Medicinal Chemistry:

10h

Basic terminology of medicinal chemistry, Types of disease, Drug nomenclature, classification of drugs, enzymes and bio-receptors, molecular messengers, synthesis of analgesic, antipyretic, antibacterial, antimalarial, anticancer, antidiabetic and antiviral drugs. Concepts of API and Bulk drug synthesis.

References:

1. Analytical Chemistry by David Krupadanam, Universities Press (India) Limited
2. D.A. Skoog, F.J. Holler, T.A. Nieman, Principles of Instrumental Analysis, EngageearningIndia Ed.
3. D. A. Skoog, D.M. West, F.J. Holler, Fundamentals of Analytical Chemistry 6thEd., Saunders College Publishing, Fort worth (1992).
4. Willard, H.H., Merritt, L.L., Dean, J. & Settoe, F.A. Instrumental Methods of Analysis. 7thEd. Wadsworth Publishing Co. Ltd., Belmont, California, USA, 1988.
5. Harris, D. C. Quantitative Chemical Analysis, W. H. Freeman. 2007.
6. Dean, J. A. Analytical Chemistry Notebook, McGraw Hill.
7. Day, R. A. & Underwood, A. L. Quantitative Analysis, Prentice Hall of India.
8. Freifelder, D. Physical Biochemistry 2nd Ed., W.H. Freeman and Co., N.Y. USA, 1982.
9. Cooper, T.G. The Tools of Biochemistry, John Wiley and Sons, N.Y. USA. 16, 1977.
10. Vogel, A. I. Vogel's Qualitative Inorganic Analysis 7th Ed., Prentice Hall.
11. Vogel, A. I. Vogel's Quantitative Chemical Analysis 6th Ed., Prentice Hall.
12. Robinson, J.W. Undergraduate Instrumental Analysis 5th Ed., Marcel Dekker, Inc, New York (1995).
13. Analytical Chemistry 7th edition by Gary D. Christian (2004).
14. B. K. Sharma, Industrial Chemistry (including Chemical Engineering). Edn. (1997).
15. M.N Sastry, Separation Methods, Paperback (2004), Himalaya Publications.
16. Usharani Analytical Chemistry Paperback (2000) Narosa Publications.
17. Fundamentals of Molecular Spectroscopy, Banwell and McCash.
18. Introduction to Molecular Spectroscopy, G.M. Barrow.
19. Absorption Spectroscopy of Organic Compounds, J.R. Dyer.
20. Biochemistry: Hames and Hooper.
21. Introduction to Spectroscopy, Pavia Lampman Kriz.



22. Pharmaceutical analysis, Watson
23. NMR in Chemistry- A multinuclear introduction, William Kemp.
24. Organic Spectroscopy, William Kemp.
25. Spectroscopy of organic compounds, P.S. Kalsi.
26. Structural methods in Inorganic chemistry, E.A.V Ebsworth.
27. Organic Spectroscopy, LDS Yadav
28. Organic Spectroscopy, Y.R. Sharma
29. Molecular Spectroscopy – Arhuldas
30. Medicinal chemistry-Ashutosh Kar

Laboratory Course (30h)

1. Chromatography

Thin layer chromatography: Determination of purity of a given sample, monitoring the progress of chemical reactions and column chromatographic separations, identification of unknown organic compounds by comparing the R_f values of known standards, and preparative TLC for separation of mixtures.

Separation / Purification by column chromatography: Separation of isomeric mixtures using column chromatography with simultaneous monitoring of separation of compounds using TLC.

2. Interpretation of spectral data

Identification of unknown organic compounds by interpretation of IR, ^1H NMR, ^{13}C NMR and mass spectra.

3. ChemDraw and ChemSketch: Molecular structure drawing with 3D geometry, drawing of chemical reactions with mechanism, Chemical analysis.

4. HPLC: Demonstration of analysis of purity of organic compound by using HPLC (Virtual)

5. Organic synthesis: Basic synthetic reactions: Oxidation, Reduction, cyclization and condensation reactions. Total synthesis of chromone, coumarin and quinoline based natural products. Isolation of Natural products.

References:

1. Practical organic chemistry by Mann & Saunders
2. Text book of practical organic chemistry by Vogel
3. Chromatography: Principles and Instrumentation (Chemical Analysis)
4. Practical chemistry by V.K Ahluwalia, Sunitha Dhingra, Adarsh Gulati.



5. Text book of practical organic chemistry by Vogel
6. The systematic identification of organic compounds by Shriner et.al
7. Analytical chemistry by G N David Krupadanam et.al
8. Advanced practical medicinal chemistry by Ashutoshkar
9. Pharmaceutical drug analysis by Ashutoshkar
10. Quantitative analysis of drugs in pharmaceutical formulations by P D Sethi
11. Practical pharmaceutical chemistry part-1 and part-2 by A H Beckett and J B Stenlake
12. Organic Spectroscopy by JagMohan.

8. Kinetics and Mechanism of Chemical Transformations, J. Rajaraman and J. Kuriacose, McMillan
9. Introduction to Electrochemistry, S. Glasstone
10. Modern Electrochemistry, J. O. M. Bockris & A. K. N. Reddy, Plenum
11. Principles of physical chemistry, Samuel H. Maron and Carl F. Prutton, Oxford & IBH
12. The Physical Basis of Organic Chemistry by Howard Maskill, Oxford University Press (New York)
13. Chemical Kinetics and Reaction Mechanisms, J. H. Espenson, McGraw Hill
14. Physical Organic Chemistry, N. S. Isaacs, ELBS
15. Elementary Quantum Chemistry, F. L. Pilar, McGraw Hill.
16. Quantum Chemistry – D.A. McQuarrie Viva Publications

Paper-IV: CH 104 (ANALYTICAL TECHNIQUES and SPECTROSCOPY- I)

ASP 01: Techniques of Chromatography

ASP 02: NMR spectroscopy-I (^1H NMR)

ASP 03: Rotational and Vibrational spectroscopy

ASP 04: Electronic spectroscopy

ASP-01: Techniques of Chromatography

15 hrs

- i. Introduction, Classification of chromatographic techniques, differential migration rates, partition ratio, retention time, relation between partition ratio and retention time, capacity factor, selectivity factor. Efficiency of separation- resolution, diffusion, plate theory and rate theory.
- ii. **GC:** Principle, instrumentation, detectors- TCD, FID, ECD. Derivatisation techniques, PTGC.
- iii. **HPLC:** Principle, instrumentation, detectors- UV detectors, Photodiode array detector, fluorescence detector.
- iv. Applications: Methods of quantitation for GC and HPLC: GC analysis of hydrocarbons in a mixture, GC assay of methyl testosterone in tablets, atropine in eye drops. HPLC assay of paracetamol and aspirin in tablets.

ASP 02: NMR spectroscopy-I (^1H NMR)

15 hrs

^1H NMR spectroscopy: Magnetic properties of nuclei, Principles of NMR Instrumentation, CW and pulsed FT instrumentation, equivalent and non equivalent protons, enantiotopic and diastereotopic protons, Chemical shifts, factors affecting the chemical shifts, electronegativity and anisotropy, shielding and deshielding effects, Signal integration, Spin-spin coupling: vicinal, germinal and long range, Coupling constants and factors affecting coupling constants.

Applications of ^1H NMR spectroscopy: Reaction mechanisms (cyclic bromonium ion, electrophilic and nucleophilic substitutions, carbocations and carbanions), E, Z isomers, conformation of cyclohexane and decalins, keto-enol tautomerism, hydrogen bonding, proton exchange processes (alcohols, amines and carboxylic acids), C-N rotation. Magnetic resonance imaging (MRI). ^1H NMR of organic molecules and metal complexes: ethyl acetate, 2-butanone, mesitylene, paracetamol, aspirin, ethylbenzoate, benzyl acetate, 2-chloro propionic acid, $[\text{HNi}(\text{OPeEt}_3)_4]^+$, $[\text{HRh}(\text{CN})_5]$ ($\text{Rh } I=1/2$), $[\text{Pt}(\text{acac})_2]$.

ASP 03: Rotational, Vibrational and Raman spectroscopy**15 hrs**

a) Microwave Spectroscopy: Classification of molecules based on moment of inertia. Diatomic molecule as rigid rotator and its rotational energy levels. Selection rules (derivation not required). Calculation of bond lengths from rotational spectra of diatomic molecules. Isotope effect on rotational spectra. Calculation of atomic mass from rotational spectra. Brief description of microwave spectrometer.

b) Vibrational Spectroscopy. Vibrational energy levels of diatomic molecules, selection rules (derivation not required). Calculation force constant from vibrational frequency. Anharmonic nature of vibrations. Fundamental bands, overtones and hot bands, Fermi Resonance. Vibrationrotation spectra diatomic molecules. Vibrations of poly atomic molecules. Normal modes of vibration, concept of group frequencies. Characteristics of vibrational frequencies of functional groups; Stereochemical effects on the absorption pattern in carbonyl group, cis-trans isomerism and hydrogen bonding. Isotopic effect on group frequency. IR spectra of metal coordinated NO_3^- , SO_4^{2-} and CO_3^{2-} ions.

c) Raman Spectroscopy- Classical and Quantum theories of Raman effect. Rotational Raman and Vibrational Raman spectra, Stokes and anti- Stokes lines. Complementary nature of IR and Raman spectra.

ASP 04: Electronic spectroscopy**15 hrs**

Electronic spectroscopy: Electronic spectra: Elementary energy levels of molecules-selection rules for electronic spectra; types of electronic transitions in molecules. Chromophores: Congugated dienes, trienes and polyenes, unsaturated carbonyl compounds, Benzene, mono substituted derivative (Ph-R), di substituted derivative ($\text{R-C}_6\text{H}_4\text{-R}$) and substituted benzene derivatives ($\text{R-C}_6\text{H}_4\text{-COR}$), Woodward-Fieser rules. Polynuclear aromatic compounds (Biphenyl, stilbene, naphthalene, anthracene, phenanthrene and pyrene). Heterocyclic systems. Absorption spectra of charge transfer complexes. Solvent and structural influences on absorption maxima, stereochemical factors. Cis-trans isomers, and cross conjugation. Beer's law application to mixture analysis and dissociation constant of a weak acid.

References:

1. Fundamentals of Molecular Spectroscopy, Banwell and McCash.
2. Introduction to Molecular Spectroscopy, G.M. Barrow.
3. Absorption Spectroscopy of Organic Compounds, J.R. Dyer.
4. Biochemistry: Hames and Hooper.
5. Introduction to Spectroscopy, Pavia Lampman Kriz.
6. Pharmaceutical analysis, Watson
7. NMR in Chemistry- A multinuclear introduction, William Kemp.
8. Organic Spectroscopy, William Kemp.
9. Spectroscopy of organic compounds, P.S. Kalsi.
10. Structural methods n Inorganic chemistry, E.A.V Ebsworth.
11. Organic Spectroscopy, LDS Yadav
12. Organic Spectroscopy, Y.R. Sharma
13. Molecular Spectroscopy – Arhuldas
14. Vibrational spectroscopy – D.N. Satyanarayana

Practicals:**Paper CH 151: Inorganic chemistry practicals: 6 hrs/week****I. Calibrations:**

- (i) Calibration of weights.
- (ii) Calibration of pipettes.
- (iii) Calibration of standard flasks.
- (iv) Calibration of burette.

II. EDTA back-titrations:

- (i) Estimation of Ni^{2+} .
- (ii) Estimation of Al^{3+} .

III. EDTA substitution titrations:

Estimation of Ca^{2+} .

IV. Redox Titrations

- (i) Estimation of Ferrocyanide and Ferricyanide in a mixture

V. Preparation of complexes:

- (i). Hexaammine nickel (II) chloride.
- (ii). Tris (acetylacetonato) manganese.
- (iii). Tris (ethylenediamine) nickel (II) thiosulphate.
- (iv). Mercury tetrathiocyanato cobaltate (II).
- (v). Chloro pentaammine cobalt (III) chloride
- (vi). Tetrammine copper (II) sulphate and estimation of NH_3 and calculation of % purity.
- (vii) One component gravimetric estimations (Use of sintered glass crucible)
 - a) Estimation of Zn^{2+}
 - b) Estimation of Ba^{2+} (as BaSO_4)

Paper CH 152 Organic Chemistry Lab course**6 hours/ week**

Synthesis of the following compounds: p-Bromoacetanilide, p- Bromoaniline, 2,4,6-tribromoaniline, 1,3,5-tribromobenzene, aspirin, tetrahydrocarbazole, 7-hydroxy-4-methyl coumarin, m-dinitrobenzene, m-nitroaniline, hippuric acid, azlactone, anthracene-maleic anhydride adduct, Phthalimide, 2,4-dihydroxyacetophenone

References.

1. Text book of practical organic chemistry, Vogel
2. Text book of practical organic chemistry, Mann and Saunders.

Paper 153 Physical Chemistry Lab course: 6 hrs / week**Physical properties:**

Data analysis I: Significant figures, Precision and accuracy

Distribution:

- ☐ Distribution of acetic acid between n-butanol and water
- ☐ Distribution of iodine between hexanes and water

Chemical kinetics:

- ☐ Acid-catalyzed hydrolysis of methyl acetate
- ☐ Peroxydisulphate- I^- reaction (overall order)
- ☐ Oxidation of iodide ion by hydrogen peroxide- iodine clock reaction

Conductometry:

- ☐ Titration of strong acid vs strong base
- ☐ Titration of weak acid vs strong base
- ☐ Determination of cell constant
- ☐ Determination of dissociation constant of a weak acid

Potentiometry:

- ☐ Titration of strong acid vs strong base
- ☐ Titration of weak acid vs strong base
- ☐ Determination of dissociation constant of a weak acid
- ☐ Determination of single electrode potential

Polarimetry:

- ☐ Determination of specific rotation of sucrose
- ☐ Acid-catalyzed hydrolysis of sucrose (inversion of sucrose)

Adsorption and others:

- ☐ Adsorption of acetic acid on animal charcoal or silica gel
- ☐ Determination of critical solution temperature of phenol-water system
- ☐ Effect of added electrolyte on the CST of phenol-water system

Determination of **molecular weight of a polymer by viscometry**.

References:

1. Senior Practical Physical Chemistry: B.D. Khosla, V.C. Garg and A. Khosla
2. Experimental Physical Chemistry: V. Athawale and P. Mathur.
3. Practical Physical Chemistry: B. Vishwanathan and P.S. Raghavan.
4. Practical in Physical Chemistry: P.S. Sindhu
5. Advanced Practical Physical chemistry: J.B. Yadav
6. Vogel Text book of Quantitative Analysis, 6th edition, Pearson education Ltd. 2002.

SEMESTER –II

(Semester-I and Semester-II syllabus is common for all specializations i.e., Inorganic-Analytical, Organic, Physical, Chemistry (Pharmacoinformatics) and Physical- Organic.)

Paper CH 201 INORGANIC CHEMISTRY

IC 05: Reaction mechanisms of transition metal complexes

IC 06: Bonding in metal complexes-II

IC 07: Metal clusters

IC 08: Biocoordination chemistry

Teaching hours/week-4

Marks-80

IC-05: Reaction mechanisms of transition metal complexes:

15 hrs

Ligand substitution reactions:

Energy profile of a reaction – Transition state or Activated Complex. Types of substitution reactions (SE, SN, SN¹, SN²). Langford and Grey classification – A mechanism, D-Mechanism, I_a, I_d, and Intimate mechanism.

Ligand substitution reactions in octahedral complexes:

Aquation or Acid hydrolysis reactions, Factors effecting Acid Hydrolysis, Base Hydrolysis, Conjugate Base Mechanism, Evidences in favour of SN¹CB Mechanism.

Substitution reactions with out Breaking Metal-Ligand bond. Anation reaction

Ligand Substitution reactions in Square-Planar complexes: Mechanism of Substitution in Square-Planar complexes- Trans-effect, Trans-influence, Grienberg's Polarization theory and Π - bonding theory – Applications of Trans-effect in synthesis of Pt (II) complexes.

Electron Transfer Reactions (or Oxidation-Reduction Reactions) in Coordination compounds:

Mechanism of One-electron Transfer Reactions: Atom (or group) Transfer or Inner Sphere Mechanism, Direct electron Transfer or Outer Sphere Mechanism. Factors affecting direct electron transfer reactions, Cross reactions and Marcus-Hush theory.

IC-06: Bonding in Metal Complexes – II:

15 hrs

Free ion terms and Energy levels: Configurations, Terms, States and Microstates – Formula for the calculation of Microstates pⁿ and dⁿ configurations – L-S (Russel-Saunders) coupling scheme – j-j coupling scheme – Determination of terms for various pⁿ and dⁿ configurations of metal ions. Hole formalism – Energy ordering of terms (Hund's rules) Inter – electron repulsion Parameters (Racah parameters) – Spin-Orbital coupling parameters. Effect of weak cubic crystal fields on S,P,D and F terms- Orgel Diagrams.

IC-07: Metal Clusters:

15 hrs

Carbonyl clusters: Factors favouring Metal-Metal bonding – Classification of Clusters –

Low Nuclearity Clusters : M₃ and M₄ clusters, structural patterns in M₃(CO)₁₂ (M=Fe,Ru,Os) and M₄(CO)₁₂ (M=Co,Rh,Ir) Clusters. Metal carbonyl scrambling – High Nuclearity clusters M₅, M₆, M₇, M₈ and M₁₀ Clusters-, Polyhedral skeletal electron pair theory and Total Electron Count theory – Capping rule – Structural patterns in

[Os₆(CO)₁₈]²⁻, [Rh₆(CO)₁₆], {Os₇(CO)₂₁}, {Rh₇(CO)₁₆}³⁻, [Os₈(CO)₂₂]²⁻, [Os₁₀C(CO)₂₄]²⁻ and [Ni₅(CO)₁₂]²⁻.

Metal Halide clusters: Major structural types in Dinuclear Metal-Metal systems – Edge sharing Bioctahedra, Face sharing Bioctahedra, Tetragonal prismatic and Trigonal antiprismatic structures -. Structure and bonding in $[\text{Re}_2\text{Cl}_8]^{2-}$ and Octahedral halides of $[\text{Mo}_6(\text{Cl})_8]^{4+}$ and $[\text{Nb}_6(\text{Cl})_{12}]^{2+}$. Trinuclear halides of Re(III). Hoffman's Isolobal analogy and its Structural implications. Boranes, carboranes, STYX Rule. Stereo chemical non-rigidity in $[\text{Rh}_4(\text{CO})_{12}]$ and $[\text{Fe}_2(\text{Cp})_2(\text{CO})_4]$.

IC-08: Bio coordination chemistry:

15 hrs

Metal ions in Biological systems: Brief survey of metal ions in biological systems. Effect of metal ion concentration and its physiological effects. Basic principles in the biological selection of elements.

Oxygen transport and storage: Hemoglobin (Hb) and Myoglobin (Mb) primary, secondary, tertiary and quarternary structures and non-covalent bonds present in them. Oxygenation equilibria for Mb and Hb. Factor effecting oxygenation equilibria. Cooperativity and its mechanism. Spin state of iron. Spatial and electronic aspects of dioxygen binding. Allosteric models (T and R states). Role of globin. Transport of NO and CO₂. Hemocynin (Hc) and Hemerythrin (Hr): Introduction-structure of active sites with oxygen and without oxygen. Comparison of Hemerythrin and Hemocyanin with hemoglobin.

Photosynthesis: Structural aspects of Chlorophyll. Photo system I and Photo system II.

Vitamin B₆ model systems: Forms of vitamin B₆ with structures. Reaction mechanisms of (1) Transamination (2) Decarboxylation and (3) Dealdolization in presence of metal ions.

References:

1. Inorganic Reaction Mechanisms. M.L.Tobe and John Burgess, Addison Wesley Longman (1999).
2. Metal ions in Reaction Mechanisms. K.Veera Reddy. Golgotia Publications (P) Ltd
3. Mechanisms of Reactions in Transition Metal Sites. Richard A Henderson, Oxford Science Publications, London (1993).
4. Inorganic Reaction Mechanisms, F.Basolo and R.G.Pearson, New York (1967).
5. Advanced Inorganic Chemistry. F.A.Cotton, G.Wilkinson, C.A.Murillo and M.Bochmann, 6 Th Edition, Wiley Interscience, N.Y (1999)
6. Inorganic Chemistry, J.E.Huheey, K.A.Keiter and R.L.Keiter 4th Edition Harper Cottens College Publications (1993).
7. Inorganic Biochemistry Edited by G.L.Eichorn, Volume 1 Elsevier (1982).
8. The Chemistry of Metal Cluster Complexes. D.F.Shriver, H.D.Kaerz and R.D.Adams (Eds), VCH, NY (1990).
9. Inorganic Chemistry, Keith F.Purcell and John C.Kotz, Holt-Saunders International Editions, London (1977).
10. Bioinorganic Chemistry, I.Bertini, H.B.Gray, S.J.Lippard and S.J.Valentine, Viva Low-Priced Student Edition, New Delhi (1998).
11. Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, W.Kain and B.Schwederski, John Wiley and Sons, NY (1999).

Paper-II: CH 202 T (Organic Chemistry)

OC-05: Reaction mechanism-II

OC-06: Pericyclic reactions-I

OC-07: Photochemistry

OC-08: Reactive intermediates and molecular rearrangements

OC-05: Reaction mechanism-II**15 hrs**

Nucleophilic Aromatic substitution: Aromatic Nucleophilic substitution: $S_N1(Ar)$, $S_N2(Ar)$, and benzyne mechanisms; evidence for the structure of benzyne. Von Richter rearrangement. Definition and types of ambident nucleophiles.

Neighbouring group participation: Criteria for determining the participation of neighbouring group. Enhanced reaction rates, retention of configuration, isotopic labeling and cyclic intermediates. Neighbouring group participation involving Halogens, Oxygen, Sulphur, Nitrogen, Aryl, Cycloalkyl groups, σ and π - bonds. Introduction to nonclassical carbocations.

Electrophilic substitution at saturated carbon and single electron transfer reactions.

Mechanism of aliphatic electrophilic substitution. S_E1 , S_E2 , and S_{Ei} . SET mechanism.

OC-06 Pericyclic reactions**15 hrs.**

Introduction, Classification of pericyclic reactions,

Electrocyclic reactions: con rotation and dis rotation. Electrocyclic closure and opening in $4n$ and $4n+2$ systems.

Cycloaddition reactions: suprafacial and antarafacial additions in $4n$ and $4n+2$ cycloadditions.

Sigmatropic reactions: $[i, j]$ shifts- suprafacial and antarafacial shifts, Cope and Claisen rearrangement reactions.

Approaches for the interpretation of mechanism of pericyclic reactions: Aromatic Transition States (ATS)/Perturbation Molecular Orbitals (PMO) approach-Concept of Huckel –Möbius aromatic and antiaromatic transition states. Framing Woodward-Hofmann selection rules for all the pericyclic reactions by ATS approach. Solving problems based on ATS approach.

Molecular orbitals: ethylene, 1, 3-butadiene, 1, 3, 5-hexatriene, allyl cation, allyl radical, pentadienyl cation, pentadienyl radical.

Frontier Molecular Orbital (HOMO-LUMO) approach-concept: Framing Woodward-Hofmann selection rules for all the pericyclic reactions by Frontier Molecular Orbital (FMO) approach. Solving problems based on FMO approach.

Conservation of orbital symmetry: (Correlation Diagrams) approach- for electrocyclic and cycloadditions & cycloreversions.

OC-07 Photochemistry**15hrs**

Photochemistry: Photochemistry of $\pi-\pi^*$ transitions: Excited states of alkenes, cis-trans isomerisation, and photo stationary state. Photochemistry of 1,3-butadiene Electrocyclisation and sigmatropic rearrangements, di- π methane rearrangement. Intermolecular reactions, photocycloadditions, photodimerisation of simple and conjugated olefins. Addition of olefins to α , β -unsaturated carbonyl compounds. Excited states of aromatic compounds, Photoisomerisation of benzene.

Photochemistry of ($n-\pi^*$) transitions: Excited states of carbonyl compounds, homolytic cleavage of α - bond, Norrish type I reactions in acyclic and cyclic ketones and strained cycloalkane diones.

Intermolecular abstraction of hydrogen: photoreduction-influence of temperature, solvent, nature of hydrogen donor and structure of the substrate.

Intramolecular abstraction of hydrogen: Norrish type II reactions in ketones, esters and 1,2 diketones, Addition to carbon-carbon multiple bonds, Paterno-Buchi reaction,

Photochemistry of nitrites-Barton reaction.

OC-08: Reactive intermediates and Molecular rearrangements 15 hrs

Reactive Intermediates: Generation, detection, structure, stability and reactions of carbocations, carbanions, carbenes, nitrenes and free radicals.

Molecular rearrangements: Definition and classification. Molecular rearrangements involving 1) electron deficient carbon: Wagner- Meerwein, Pinacol-Pinacolone, Allylic and Wolf rearrangement. 2) electron deficient Nitrogen: Hofmann, Lossen, Curtius, Schmidt and Beckmann rearrangements 3) electron deficient Oxygen: Baeyer-Villiger oxidation. 4) Base catalysed rearrangements: Benzilic acid, Favorski, Transannular, Sommelet-Hauser and Smiles rearrangement

References:

1. Stereochemistry of Carbon compounds by Ernest L Eliel / Samuel H. Wilen
2. Stereochemistry of organic compounds – Principles and Applications by D Nasipuri
3. The third dimension in organic chemistry, by Alan Bassindale
4. Stereochemistry: Conformation and Mechanism by P S Kalsi
5. Stereochemistry by V M Potapov
6. Advanced Organic Chemistry by Jerry March
7. Mechanism and Structure in Organic Chemistry S. Mukerjee
8. Organic chemistry Vol.I and II by I.L.Finar
9. Comprehensive organic chemistry Vol.5 D.H.R.Barton and W.D. Ollis

Paper CH 203 PHYSICAL CHEMISTRY

PC-05: Thermodynamics-II & Statistical Thermodynamics

PC-06: Photochemistry-I

PC-07: Quantum Chemistry-II

PC-08: Solid state chemistry

PC-05: Thermodynamics-II & Statistical Thermodynamics

15 hrs

Ideal solutions. Thermodynamic properties of ideal solutions. Mixing quantities. Vapour pressure -Raoult's law. Thermodynamic properties of ideally dilute solutions. Vapour pressure- Henry's law.

Nonideal systems. Concept of fugacity, fugacity coefficient. Determination of fugacity. Non ideal solutions. Activities and activity coefficients. Standard-state conventions for non ideal solutions. Determination of activity coefficients from vapour pressure measurements. Activity coefficients of nonvolatile solutes using Gibbs-Duhem equation.

Multicomponent phase equilibrium: Vapour pressure lowering, freezing point depression and boiling point elevation

Statistical Thermodynamics:

Partition Functions: Concepts of distribution and probability, Boltzmann distribution law. Interpretation of partition functions- translational, rotational, vibrational and electronic partition functions. Relationship between partition functions and thermodynamic functions (only S & G).

PC-06: Photochemistry –I**15 hrs**

Electronic transitions in molecules. The Franck Condon principle. Electronically excited molecules- singlet and triplet states. Radiative life times of excited states-theoretical treatment. Measured life times. Quantum yield and its determination. Experimental set up of a photochemical reaction. Actinometry-ferrioxalate and uranyl oxalate actinometers – problems. Derivation of fluorescence and phosphorescence quantum yields. E-type delayed fluorescence- evaluation of triplet energy splitting (ΔE_{ST}). Photophysical processes- photophysical kinetics of unimolecular reactions. Calculation of rate constants of various photophysical processes-problems, State diagrams

Photochemical primary processes. Types of photochemical reactions- electron transfer, photodissociation, addition, abstraction, oxidation and isomerization reactions with examples. Effect of light intensity on the rates of photochemical reactions. Photosensitization. Quenching-Stern-Volmer equation. Introduction to fast reactions- Principle of flash photolysis.

PC-07: Quantum chemistry-II**15 hrs**

Cartesian, Polar and spherical polar coordinates and their interrelations.

Schrodinger equation for the hydrogen atom- separation into three equations. Hydrogen like wave functions. Radial and angular functions. Quantum numbers n , l and m and their importance. The radial distribution functions. Hydrogen like orbitals and their representation. Polar plots, contour plots and boundary diagrams.

Many electron systems. Approximate methods. The variation method-variation theorem and its proof. Trial variation function and variation integral. Examples of variational calculations. Particle in a box. Construction of trial function by the method of linear combinations. Variation parameters. Secular equations and secular determinant.

Bonding in molecules. Molecular orbital theory-basic ideas. Construction of MOs by LCAO, H_2^+ ion. The variation integral for H_2^+ ion. Detailed calculation of Wave functions and energies for the bonding and antibonding MOs. Physical picture of bonding and antibonding wave functions. Energy diagram. The MO wave function and the energy of H_2 molecule MO by LCAO method and Valence bond method (detailed calculations not required)-comparison of MO and VB models.

PC-08: Solid state chemistry**15 Hrs**

Electronic properties of metals, insulators and semi-conductors: Electronic structure of solids, Band theory, band structure of metals, insulators and semi-conductors. Electrons, holes and Excitons. The temperature dependence of conductivity of extrinsic semi-conductors. Photo conductivity and photovoltaic effect – p-n junctions.

Superconductivity: Occurrence of superconductivity. Destruction of superconductivity by magnetic fields – Meissner effect. Types of superconductors. Theories of super conductivity – BCS theory.

High temperature superconductors: Structure of defect perovskites. High T_c superconductivity in cuprates. Phase diagram of Y-Ba-Cu-O system. Crystal structure of $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$. Preparation of 1-2-3 materials. Origin of high T_c superconductivity.

Nanoparticles and their applications:

Introduction to nanoparticles. Reduced dimensionality in solids – zero dimensional systems, fullerenes, quantum dots. One dimensional systems, carbon nano tubes, preparation of nano particles –top down and bottom up methods. Preparation of nanomaterials- – sol gel methods, and chemical vapour deposition method; thermolysis. Characterization of nanoparticles – experimental methods – powder X-ray diffraction, transmission electron microscopy (TEM), and atomic force microscopy (AFM) (detailed theory and instrumentation are not required). Optical properties of nanoparticles, Applications of nanoparticles.

References:

1. Atkin's Physical Chemistry, Peter Atkins and Julio de Paula, Oxford University press
2. Physical Chemistry, Ira N. Levine, McGraw Hill
3. Physical Chemistry-A Molecular approach, D.A. McQuarrie and J.D. Simon, Viva Books Pvt Ltd
4. Molecular Thermodynamics, D.A. McQuarrie and J.D. Simon, University Science Books
5. Quantum Chemistry, Ira N. Levine, Prentice Hall
6. Introduction to Quantum Chemistry, A.K. Chandra, Tata McGraw Hill
7. Introduction to Solids, Leonid V. Azaroff, Tata McGraw Hill
8. Solid state Chemistry, D.K. Chakrabarthy, New Age International
9. Solid state Chemistry and its applications, A.R. West, Plenum.
10. Fundamentals of Photochemistry, K.K.Rohtagi-Mukherji, Wiley-Eastern
11. Molecular Photochemistry, N.J. Turro, Benjamin
12. Photochemistry, R.P.Kundall and A. Gilbert, Thomson Nelson
13. Essentials of Molecular Photochemistry by A. Gilbert and J. Baggott, Blackwell Scientific Publications.
14. Organic Photochemistry by J.M.Coxon and B.Halton, Cambridge University press.
15. Introductory Photochemistry by A.Cox and T.J.Kemp. McGraw-Hill, London.
16. Principles of the Solid State, H. V. Keer, New Age International
17. Elements of Physical Chemistry by Peter Atkins and Julio de Paula, Oxford University Press
18. Elements of Statistical Thermodynamics, L. K. Nash, Addison – Wesley
19. Introduction to Statistical Thermodynamics, T. L. Hill, Addison Wiley
20. Statistical Thermodynamics, M. C. Gupta, New Age International
21. Quantum Chemistry, D.A. McQuarrie, Prentice Hall
22. Elementary Quantum Chemistry, F. L. Pilar, McGraw Hill.
23. Nanostructured Materials and Nanotechnology, edited by Hari Singh Nalwa, Academic Press
24. Self-Assembled Nanostructures, Jin Zhang, Zhong-lin Wang, Jun Liu, Shaowei Chen & Gan-Yu-Liu, Kluwer Academic/Plenum
25. Introduction to Nanotechnology, Charles P. Poole Jr, F. J. Owens, Wiley India Pvt. Ltd.
26. The physics and chemistry of solids by Stephen Elliott, Wiley Publishers.
27. Introductory Photochemistry by A.Cox and T.J.Kemp. McGraw-Hill, London.

Paper-IV: CH 204 (ANALYTICAL TECHNIQUES and SPECTROSCOPY - II)

ASP-05: Electro and thermal analytical Techniques.

ASP-06: NMR- II

ASP-07: Mass Spectroscopy

ASP-08: Photoelectron & ESR spectroscopy

ASP-05: Electro and thermal Analytical Techniques**15 hrs****I: Types and Classification of Electro analytical Methods:**

a) D.C Polarography: Instrumentation - Dropping mercury electrode- -polarogram. Types of Currents: Residual, Migration, Limiting. Two and Three electrode assemblies. Ilkovic equation (derivation not necessary) and its consequences. Applications of polarography in qualitative and quantitative analysis. Analysis of mixtures. Application to inorganic and organic compounds. Determination of stability constants of complexes.

b) Brief account of following techniques and their advantages over conventional d.c.polarography.

(i) A.C.polarography (ii) Square-wave polarography (iii) Pulse polarography (iv) Differential pulse polarography

c) Amperometric titrations: Principle, Instrumentation. Types and applications of amperometric titrations. Determination of SO_4^{2-} , metal ions viz., Mg^{2+} , Zn^{2+} , Cu^{2+} and other substances.

d) Cyclic Voltammetry: Principle, instrumentation, Applications. Cyclic voltammetric study of insecticide parathion.

II: Thermal Analysis: Thermal techniques-Introduction, types of thermo analytical methods. Thermogravimetry principle and applications of thermogravimetry, differential thermal analysis- principle and applications of DTA. Differential scanning calorimetry. DSC: Principle, and application of DSC.

ASP 06: NMR spectroscopy-II (^1H , ^{19}F and ^{31}P NMR)**15 hrs**

^1H , ^{19}F , ^{31}P and solid state NMR spectroscopy: First order and non first order spectra e.g., AX, AX_2 , AX_3 , A_2X_3 , AMX and AB, ABC. Simplification of complex spectra: increased field strength, deuterium exchange, Lanthanide shift reagents and double resonance techniques. Discrimination of enantiomers by use of chiral NMR solvents (CSAs), chiral lanthanide shift reagents and Mosher's acid. Nuclear Overhauser enhancement (NOE). Fluxional molecules bullvalene, $[\eta^5\text{-C}_5\text{H}_5\text{M}]$, $[\eta^5\text{-(C}_5\text{H}_5)_2\text{ Ti } \eta^1\text{-(C}_5\text{H}_5)_2]$ and $[\eta^4\text{C}_8\text{H}_8\text{Ru(CO)}_3]$.

^{19}F NMR spectroscopy: ^{19}F chemical shifts, coupling constants. Applications of ^{19}F NMR involving coupling with ^{19}F , ^1H and ^{31}P : 1,2 dichloro-1,1 difluoro ethane, BrF_5 , SF_4 , PF_5 , ClF_3 , IF_5 , $\text{CF}_3\text{CH}_2\text{OH}$

^{31}P NMR spectroscopy: ^{31}P chemical shifts, coupling constants. Applications of ^{31}P NMR involving coupling with ^{31}P , ^{19}F , ^1H and ^{13}C : ATP, Ph_3PSe , P_4S_3 , H_3PO_4 , H_3PO_3 , H_3PO_2 , HPF_2 , PF_6^- , PH_3 , $[\text{Rh}(\text{PPh}_3)\text{Cl}_3]$ ($\text{Rh } I=1/2$)

Introduction to solid state NMR: Magic angle spinning (MAS). Applications of solid state NMR.

ASP 07: Mass spectrometry**15 hrs**

Origin of mass spectrum, principles of EI mass spectrometer. Types of fragments: odd electron and even electron containing neutral and charged species (even electron rule), Nitrogen rule, isotopic peaks, determination of molecular formula, metastable ion peaks. High

resolution mass spectrometry. Salient features of fragmentation pattern of organic compounds including β -cleavage, McLafferty rearrangement, retro Diels – Alder fragmentation and ortho effect. Principle of EI, CI, Fast Atom Bombardment (FAB), Secondary Ion Mass Spectrometry (SIMS), Electrospray (ESI) ionization and Matrix Assisted Laser Desorption Ionization (MALDI) methods. Introduction to principle and applications of Gas Chromatography-Mass Spectrometry (GC-MS) and Liquid chromatography-Mass Spectrometry (LC-MS) techniques.

ASP-08: Photoelectron & ESR spectroscopy

15 hrs

Photoelectron Spectroscopy

Principle and Instrumentation, Types of Photoelectron Spectroscopy – UPS & XPS. Binding Energies, Koopman's Theorem, Chemical Shifts. Photoelectron Spectra of Simple Molecules: N_2 , O_2 , F_2 - Vibrational Structure of PES Bands, Potential energy curves, Interpretation of Vibrational spectral data for ionized (M^+) species, Prediction of Nature of Molecular Orbitals. ESCA in qualitative analysis, Principles of Auger electron spectroscopy.

Electron Spin Resonance

Introduction, principle, instrumentation, selection rules, interpretation of Lande's factor 'g'. Hyperfine and super hyperfine Coupling. Anisotropy in 'g' values and hyperfine coupling constants. Zero field splitting, Kramer's degeneracy and quadrupolar interactions. Study of free radicals and transition metal complexes. Evidence for covalency in complexes, ex. Cu(II) Bissalicylaldimine, Bis-acetylacetonatovanadyl(II) and hexachloroiridium(IV) complexes.

References:

1. Spectroscopic identification of organic compounds by R.M. Silverstein and F.X. Webster.
2. Organic spectroscopy by William Kemp
3. Mass Spectrometry for Chemists and biochemists by M. Rose and R.A. W. Johnstone
4. Spectroscopic methods in organic chemistry by D.H. Williams and I. Fleming
5. Practical Pharmaceutical Chemistry by A. H. Beckett and J.B. Stenlake
6. Biological Mass Spectrometry by A.L. Burlingame
7. Principles and Practice of Biological Mass Spectrometry by Chhabil Das
8. Spectroscopic identification of organic compounds by R.M. Silverstein. G.C. Bassler and T.E. Morrill
9. NMR-A multinuclear introduction by William Kemp
10. Stereochemistry of Carbon compounds by Ernest L Eliel / Samuel H. Wilen
11. Principles of Polarography, Heyrovsky.
12. Principles of Polarography, Kapoor.
13. Modern Electroanalytical methods, edited by C. Charlot, Elsevier Company.
14. Principles of Instrumental analysis, Skoog, Holler and Nieman, Harcourt Asia PTE Ltd.
15. Analytical Chemistry-An Introduction, Skoog, West, Holler and Crouch, Saunders College Publishing.
16. Principles of Instrumental Analysis, Skoog and Leary, Saunders College Publishing.
17. International series of Monographs, Vol. 53: Photoelectron Spectroscopy, Edited by D. Becker and D. Betteridge 1972.
18. Structural methods in inorganic chemistry, E.A.V. Ebsworth

Practicals:**Paper CH 251: Inorganic chemistry practicals****I. Analysis of Two component mixtures:**

- (i). Separation of Ni^{2+} and Cu^{2+} in a mixture and estimation of Ni^{2+} (gravimetric) and Cu^{2+} (volumetric).
- (ii). Separation of Fe^{2+} and Al^{3+} in a mixture and estimation of Fe^{2+} volumetrically and Al^{3+} gravimetrically.
- (iii). Separation of Ag^+ and Ca^{2+} in a mixture and estimation of Ag^+ gravimetrically and Ca^{2+} volumetrically.

II. Analysis of three component mixtures:

- (i). Separation of (Ni^{2+} and Cu^{2+}) from Mg^{2+} in the given mixture and estimation of Mg^{2+} (Gravi).

III Applied titrimetric analysis

- (i) Determination of Iron and calcium in Cement
- (ii) Determination of Calcium in calcium tablets
- (iii) Determination of alkali content in antacid

IV. Ion exchange methods of analysis:

- (i). Determination of capacity of an ion exchange resin.
- (ii). Separation of Zinc and Magnesium on an anion exchange resin and estimation of Mg^{2+} and Zn^{2+} .

Suggested Books: (For both semesters).

1. (i). Text book of Quantitative Inorganic Analysis by A.I.Vogel, 3rd edition, ELBS 1969.
- (ii). Vogel's text book of Quantitative Inorganic analysis. Jeffery et al, 4th edition, ELBS 1988.
- (iii). Vogel's text book of Quantitative Inorganic Analysis. 6th edition, Pearson education Ltd 2002.
2. Practical Inorganic chemistry By G.Marr and R.W.Rockett 1972.
3. Experimental Inorganic/Physical Chemistry – An Investigative integrated approach to Practical Project work. By Mounir A.Malati, 1999.
4. Advanced experimental Inorganic chemistry by. Ayodhya Singh.
5. Practical Inorganic Chemistry by G. Pass & H. Sutchiffe, 2nd edn John Wiley & sons

Paper CH 252: Organic Chemistry Lab 6 hours/ week**Identification of organic compounds systematic qualitative analysis:**

Physical data BP / MP, Ignition test, solubility classification, Extra elements-N,S & Halogens, (Lassaigne sodium fusion test, Beilstein test)

Functional groups tests, Preparation of crystalline derivative and determination of their m.p.s and reference to literature to identify the compounds

A minimum of **10** following compounds to be studied as unknown covering atleast one from each of the solubility classes

Glucose, benzoic acid, 2-chloro benzoic Acid, Anisic acid, p-Nitrobenzoic acid; p-Cresol, p-Chlorophenol, β -Naphthol; Aniline, o/m/p-Chloroanilines; N-Methyl aniline/N-Ethylaniline, N,N-Dimethylaniline, Benzamide, Benzaldehyde, Anisaldehyde, Acetophenone, benzophenone, Ethylbenzoate, methylbenzoate, Nitrobenzene, chlorobenzene, bromobenzene, naphthalene, biphenyl anthracene.

Identification of unknown organic compounds from their IR, UV, ^1H NMR and MS:

Analysis of recorded spectra of 6 compounds belonging to i) aromatic carboxylic acid ii) alcohols and phenols iii) aldehydes and ketones iv) amides v) esters vi) alkenes and alkynes

References

1. Text book of practical organic chemistry, Vogel
2. Text book of practical organic chemistry, Mann and Saunders.
3. Spectral identification of organic compounds Bassler, Silverstein 5th Edition

Paper CH 253: Physical Chemistry Lab: 6 hrs /week

Data analysis II: Mean and standard deviation; absolute and relative errors; linear regression; covariance and correlation coefficient.

Distribution:

- 1) Distribution of I_2 between hexanes / cyclo hexanes / CCl_4 and aq.KI solution- calculation of equilibrium constant.
- 2) Study of complex formation between ammonia and metal ion

Chemical Kinetics

- 1) Stoichiometry of peroxydisulphide- iodide reaction
- 2) Peroxydisulphide- iodide reaction: order w.r.t $[\text{I}^-]$ by isolation method
- 3) Peroxydisulphide- iodide reaction: order w.r.t $[\text{S}_2\text{O}_8^{2-}]$ by initial rate method

Conductometry:

- 1) Titration of a mixture of strong and weak acids vs strong base
- 2) Determination of the hydrolysis constant of aniline hydrochloride
- 3) Determination of solubility product

Potentiometry:

- 1) Titration of Fe^{+2} vs $\text{Cr}_2\text{O}_7^{2-}$ (redox titration)
- 2) Titration of Cl^- vs Ag^+ (precipitation titration)
- 3) Determination of solubility product

Polarimetry:

- 1) Determination of specific rotation of glucose and fructose
- 2) Enzyme catalysed inversion of sucrose

Colorimetry:

- 1) Verification of Beer's law and calculation of molar absorption coefficient using CuSO_4 and KMnO_4 solutions

pH metry:

- 1) Calibration of a pH meter and measurement of pH of different solutions
- 2) Preparation of phosphate buffers
- 3) Titration of strong acid vs strong base

References:

1. Senior Practical Physical Chemistry: B.D. Khosla, V.C. Garg and A. Khosla
2. Experimental Physical Chemistry: V. Athawale and P. Mathur.
3. Practical Physical Chemistry: B. Vishwanathan and P.S. Raghavan.
4. Practical in Physical Chemistry: P.S. Sindhu
5. Advanced Practical Physical chemistr: J.B.Yadav
6. Vogel Text book of Quantitative Analysis, 6th edition, Pearson education Ltd. 2002

(For the batch admitted during the academic year 2016-2017)

Paper-1CH (OC) 301T: Synthetic Reagents, Advanced NMR, Conformational Analysis and ORD

OC-09: Synthetic Reagents-I

OC-10: Synthetic Reagents-II

OC-11: ^{13}C NMR and 2D NMR spectroscopy

OC-12: Conformational analysis (Cyclic systems) & ORD

Paper II– CH (OC) 302T: Modern Organic Synthesis

OC-13: Asymmetric synthesis

OC-14: Synthetic strategies

OC-15: New Synthetic reactions

OC-16: New techniques and concepts in organic synthesis

Elective-3A Paper-III CH (OC) 303T (CB1): Bioorganic Chemistry

OC(CB1)-1: Carbohydrates

OC(CB1)-2: Nucleic acids and Lipids

OC(CB1)-3: Proteins and Enzymes

OC(CB1)-4: Coenzymes and Vitamins

Elective-3B: Paper-III CH (OC) 303T (CB2): Forensic Chemistry and Toxicology

OC(CB2)-5: Forensic chemistry- I

OC(CB2)-6: Forensic chemistry- II

OC(CB2)-7: Forensic Toxicology-I

OC(CB2)-8: Forensic Toxicology-II

Elective-4A Paper-IV CH (OC) 304T (CB3): Green chemistry and Organic materials

OC (CB3) - 9: Principles of Green chemistry

OC (CB3) -10: Green Synthesis

OC (CB3) -11: Organic nanomaterials

OC (CB3) -12: Supramolecular chemistry

Elective-4B Paper-IV CH (OC) 304T (CB4): Pesticides

OC (CB4) - 13: Introduction to pesticides

OC (CB4) - 14: Synthetic insecticides

OC (CB4) - 15: Natural insecticides & herbicides

OC (CB4) - 16: Fungicides, and Rodenticides

Laboratory courses:

Paper-V CH (OC) 351P: Synthesis of organic molecules, isolation of natural products and TLC.

Paper-VI CH (OC) 352P: Separation and identification of organic compounds & Column chromatography.

(For the batch admitted during the academic year 2016 -2017 under the CBCS pattern)

**Paper-1CH (OC) 301T: Synthetic Reagents, Advanced NMR,
Conformational Analysis and ORD**

OC-09: Synthetic Reagents-I

OC-10: Synthetic Reagents-II

OC-11: ^{13}C NMR and 2D NMR spectroscopy

OC-12: Conformational analysis (Cyclic systems) & ORD

OC-09: Synthetic Reagents I

15 Hrs

i)Protecting groups: a) Protection of alcohols by ether, silyl ether and ester formation
b) Protection of 1,2-diols by acetal, ketal and carbonate formation c) Protection of amines by benzyloxycarbonyl, t-butyloxycarbonyl, fmoc and triphenyl methyl groups. d) Protection of carbonyls by acetal, ketal and thiol acetal (Umpolung) groups. e) Protection of carboxylic acids by ester and ortho ester (OBO) formation.

ii) Organometallic Reagents: Preparation and application of the following in organic synthesis: 1) Organolithium 2) Organo copper reagents 3) Organoboranes in C-C bond formation 4) Organo silicon reagents: reactions involving β -carbocations and α -carbanions, utility of trimethyl silyl halides, cyanides and triflates.

iii) Carbonyl methylenation: a) Phosphorous ylide mediated olefination 1) Wittig reaction, 2) Horner-Wadsworth-Emmons reaction. b) Titanium- Carbene mediated olefination 1) Tebbe reagent, 2) Petasis reagent 3) Nysted reagent.

iv) Carbene insertions: Rh based carbene complexes, cyclopropanations.

v) C-H Activation: Introduction, Rh catalysed C-H activation.

OC-10: Synthetic Reagents II

15 Hrs

i) Oxidations: a) Oxidation of active C-H functions: DDQ and SeO_2 . b) Alkenes to diols: Prevost and Woodward oxidation c) Alcohol to carbonyls: Cr^{VI} oxidants (Jones reagent, PCC, PDC) IBX, DMP, CAN, TEMPO, TPAP, Swern oxidation d) Oxidative cleavage of 1,2-diols: Periodic acid and Lead tetra acetate.

ii) Reductions: a) Catalytic hydrogenation: Homogenous (Wilkinson's catalytic hydrogenation) and heterogeneous catalytic reduction. b) Non-metallic reductions: Diimide reduction c) Dissolving metal reductions: Birch reduction. d) Nucleophilic metal hydrides: LiAlH_4 , NaBH_4 , and their modifications. e) Electrophilic metal hydrides: BH_3 , AlH_3 and DIBAL. f) Use of tri-n-butyl tin hydride: Radical reductions.

OC-11: ^{13}C NMR and 2D NMR spectroscopy 15 Hrs

i) ^{13}C NMR spectroscopy: Introduction, Types of ^{13}C NMR spectra: uncoupled, proton-

decoupled and off-resonance decoupled (ORD) spectra. ^{13}C chemical shifts, factors affecting the chemical shifts, chemical shifts of organic compounds. Calculation of chemical shifts of alkanes, alkenes and alkynes. Homonuclear (^{13}C , ^{13}C J) and heteronuclear (^{13}C , ^1H J and ^{13}C , ^2H J) coupling. Applications of ^{13}C -NMR spectroscopy: Structure determination, stereochemistry, reaction mechanisms and dynamic processes in organic molecules. ^{13}C -NMR spectral editing techniques: principle and applications of APT, INEPT and DEPT methods.

ii) 2D-NMR spectroscopy: Principles of 2D NMR, Classification of 2D-experiments. Correlation spectroscopy (COSY) HOMOCOSY (^1H - ^1H COSY), TOCSY (Total Correlation Spectroscopy), HeteroCOSY (^1H , ^{13}C COSY, HMQC), long range ^1H , ^{13}C COSY (HMBC), Homonuclear and Heteronuclear 2D-J-resolved spectroscopy, NOESY and 2D-INADEQUATE experiments and their applications.

OC-12: Conformational analysis (Cyclic systems) & ORD 15 Hrs

Conformational analysis (Cyclic systems)

Study of conformations of cyclohexane, mono, di and tri substituted cyclohexanes, (1,3,5-trimethyl cyclohexanes and Menthols), cyclohexanone (2-alkyl and 3-alkyl ketone effect), 2-halocyclohexanones, cycloheptane. Stereo chemistry of bicyclo[3,3,0]octanes, hydrindanes, decalins and perhydroanthracenes. Conformational structures of piperidine, N-Methylpiperidine, tropine, tropine, pseudotropine, decahydroquinoline and quinolizidine. Factors governing the reactivity of axial and equatorial substituents in cyclohexanes.

(oxidation, $\text{S}_{\text{N}}2$ reaction, rearrangements, Ester hydrolysis) Stereochemistry of addition to the carbonyl group of a rigid cyclohexanone ring.

Optical Rotatory Dispersion (ORD) and CD Spectroscopy: Optical rotation, circular birefringence, circular dichroism and Cotton effect. Plain curves and anomalous curves. Empirical and semiempirical rules-The axial haloketone rule, the octant rule, Helicity rule, Exciton chirality method. Application of the rules to the study of absolute configuration and conformations of organic molecules.

Recommended Books:

1. Some modern methods of organic synthesis by W. Carruthers
2. Guidebook to organic synthesis, by R K Meckie, D M Smith & R A Atken
3. Organic Synthesis by O House
4. Organic synthesis by Micheal B Smith
5. Reagents for organic synthesis, by Fieser & Fieser, Vol 1-11 (1984)
6. Organic synthesis by Robert E Ireland
7. Handbooks of reagents for organic synthesis by Reich and Rigby, Vol-I-IV
8. Organic chemistry by Jonathan Clayden, Nick Greeves and Stuart Warren
9. Organic Reactions and their mechanisms by P.S. Kalsi
10. Organic reaction mechanisms by V.K. Ahluwalia and Rakesh Kumar Parashar
11. Spectroscopic identification of organic compounds by RM Silverstein, G C Bassler and T B Morrill
12. Organic Spectroscopy by William Kemp
13. Spectroscopic methods in Organic chemistry by DH Williams and I Fleming
14. Modern NMR techniques for chemistry research by Andrew B Derome

15. NMR in chemistry - A multinuclear introduction by William Kemp
16. Spectroscopic identification of organic compounds by P S Kalsi
17. Introduction to organic spectroscopy by Pavia
18. Carbon-13 NMR for organic chemists by GC Levy and O L Nelson
19. Nuclear Magnetic Resonance Basic principles by Atta-ur-Rahman
20. Basic one and two-dimensional NMR spectroscopy by Horst Friebolin
21. NMR spectroscopy by H.Gunther
22. Stereochemistry of organic compounds — Principles & Applications by D Nasipuri
23. Stereochemistry of Carbon compounds by Ernest L Eliel & Samuel H. Wilen
24. Stereochemistry: Conformation & Mechanism by P S Kalsi
25. The third dimension in organic chemistry, by Alan Bassendale
26. Stereo selectivity in organic synthesis by R S Ward.
27. Advanced organic chemistry. Part A Structure & Mechanism by Francis A. Corey and Richard J. Sundberg
28. Optical rotatory dispersion by C Djerassi
29. Optical rotatory dispersion and circular dichroism by P Crabbe
30. Mechanism and Structure in Organic chemistry by S Mukherjee

Paper II– CH (OC) 302T:Modern Organic Synthesis

OC-13: Asymmetric synthesis

OC-14: Synthetic strategies

OC-15: New Synthetic reactions

OC-16: New techniques and concepts in organic synthesis

OC- 13:- Asymmetric synthesis 15 Hrs

Introduction: Brief revision of classification of stereo selective reactions

Prostereoisomerism: Topicity in molecules Homotopic, stereoheterotopic (enantiotopic and diastereotopic) groups and faces- symmetry criteria.

Prochiral nomenclature: Pro chirality and Pro-R, Pro-S, Re and Si.

Conditions for stereoselectivity: Symmetry and transition state criteria, kinetic and thermodynamic control. Methods of inducing enantioselectivity.

Analytical methods: % Enantiomeric excess and diastereomeric ratio. Determination of enantiomeric excess: specific rotation, Chiral NMR; Chiral derivatizing agents, Chiral solvent, Chiral shift reagents and Chiral HPLC.

Chiral Substrate controlled asymmetric synthesis: Nucleophilic additions to chiral carbonyl compounds. 1, 2- asymmetric induction, Cram's rule and Felkin-Anh model.

Chiral auxiliary controlled asymmetric synthesis: α -Alkylation of chiral enolates, Evans' oxazolidinone, 1, 4-Asymmetric induction and Prelog's rule..

Chiral reagent controlled asymmetric synthesis: Asymmetric reductions using BINAL-H. Asymmetric hydroboration using IPC_2BH and IPCBH_2 .

Chiral catalyst controlled asymmetric synthesis: Sharpless epoxidation. Asymmetric hydrogenations using chiral Wilkinson biphosphine catalyst.

Asymmetric aldol reaction: Diastereoselective aldol reaction (achiral enolate & achiral aldehydes) its explanation by Zimmerman-Traxel model.

OC-14: Synthetic Strategies 15 Hrs

Introduction: Terminology, Target, synthon, synthetic equivalent, functional group interconversion (FGI), functional group addition. Criteria for selection of target. Linear and convergent synthesis. Retrosynthetic analysis and synthesis involving chemoselectivity, regioselectivity, reversal of polarity and cyclizations. .

Order of events: S-Salbutamol, Propoxycaïne..

One group C-C and C-X disconnections: Introduction .One group C-C disconnections in alcohols and carbonyl compounds. One group C-X disconnections in Carbonyl compounds, alcohols, ethers and sulphides.

Two group C-C and C-X disconnections : Introduction .Two group C-X disconnections in 1,1-difunctionalised, 1,2-difunctionalised and 1,3-difunctionalised compounds.

Two group C-C disconnections: Diels-Alder reaction, 1,3-difunctionalised compounds, 1,5-difunctionalised compounds, Michael addition and Robinson annulation.

Control in carbonyl condensations: oxalamide and mevalonic acid.

Strategic bond: definition, guidelines for disconnection; disconnection of C-X bonds, disconnect to greatest simplification, using symmetry in disconnection, disconnection corresponding to known reliable reaction, high yielding steps and recognizable starting materials. Retrosynthesis of Retronecene, longifoline.

OC-15: New Synthetic reactions

15 Hrs

- 1. Metal mediated C-C and C-X coupling reactions:** Suzuki, Heck, Stille, Sonogishira crosscoupling, Buchwald-Hartwig and Negishi-Kumada coupling reactions.
- 2. C=C Formation Reactions:** Shapiro, Bamford-Stevens, McMurrey reactions, Julia-Lythgoe olefination and Peterson's stereoselective olefination.
- 3. Multicomponent Reactions:** Ugi, Passerini, Biginelli, Bergman and Mannich reactions.
- 4. Ring Formation Reactions:** Pausan-Khand reaction, Nazarov cyclisation.
- 5. Click Chemistry:** Click reaction, 1,3-dipolar cycloadditions.
- 6. Metathesis:** Grubb's 1st and 2nd generation catalyst, Olefin cross coupling metathesis (OCM), ring closing metathesis (RCM), ring opening metathesis (ROM), applications.
- 7. Other important synthetic reactions:** Baylis-Hilman reaction, Eschenmoser-Tanabe fragmentation, Mitsunobu reaction, Stork-enamine reaction and Michael reactions.

OC-16: New techniques and concepts in organic synthesis 15 Hrs

- 1. Techniques in peptide synthesis:** Solid phase peptide synthesis, commonly used resins (Rink resin, Wang resin and Ellman resin, synthesis of cross linked Merrifield resin and drawbacks of solid phase synthesis.
- 2. Solid phase oligodeoxynucleotide synthesis:** Phosphotriester, phosphitetriester and phosphoramidite pathway
- 3. Oligosaccharide synthesis:** Glycosidation: cyclooxocarbeniumion, glycosyl donors and glycosyl acceptors, Kuhn glycosidation, convergent and linear oligosaccharide synthesis.
- 4. Phase Transfer catalysis:** Onium and crown ethers as PTC.
- 5. Tandem synthesis:** Tandem reactions; conjugate addition-aldol reaction, polymerization-cyclisation, electrocyclic-Diels Alder reaction.
- 6. Baldwin Rules:** Exo and Endo cyclisation, tetrahedral, trigonal and diagonal systems, favoured and disfavoured cyclisations.
- 7. Chiron approach in organic synthesis:** Nature's chiral pool, carbohydrates, amino acids, hydroxy acids, terpenes as chiral precursors. Synthesis of shikimic acid from D-arabinose, furanonycin from D-glucose, S-(-)-iphenol from S-leucine.
- 8) Determination of absolute configuration:** Mosher's method.

Recommended Books:

1. Asymmetric synthesis by Nogradi
2. Asymmetric organic reactions by J D Morrison and H S Moscher
3. Principles in Asymmetric synthesis by Robert E. Gawley & Jeffrey Aube
4. Stereo differentiating reactions by Izumi
5. Some modern methods of organic synthesis by W Carruthers
6. Guidebook to organic synthesis, by R K Meckie, D M Smith & R A Atken
7. Organic synthesis by Michael B Smith
8. Organic Synthesis-The disconnection approach by S Warren
9. Organic Synthesis by C Willis and M Willis
10. Problems on organic synthesis by Stuart Warren
11. Organic chemistry Jonathan Clayden, Nick Greeves and Stuart Warren
12. The logic of chemical synthesis by Elias James Corey and Xue-Min Cheng
13. Name reactions by Jie-Jie Li

Elective-3A

Paper-III CH (OC)303T (CB1): Bioorganic Chemistry

OC(CB1)-1: Carbohydrates**OC(CB1)-2: Nucleic acids and Lipids****OC(CB1)-3: Proteins and Enzymes****OC(CB1)-4: Coenzymes and Vitamins****OC(CB1)-1: Carbohydrates****15 Hrs**

Introduction to the importance of Carbohydrates. Types of naturally occurring sugars. Deoxy sugars, aminosugars, branched chain sugars methyl ethers and acid derivatives of sugars. Determination of configuration and determination of ring size of D-glucose and D-Fructose. Conformational analysis of monosaccharides. 4C_1 and 1C_4 conformations of D-glucose. Reactions of six carbon sugars: Ferrier, Hanesian reaction and Ferrier rearrangement. Synthesis of amino, halo and thio sugars. Structure, ring size determination of sucrose and maltose. Conformational structures of sucrose, lactose, maltose, cellobiose and gentobiose. Structure and biological functions of starch, cellulose, glycogen and chitin. Role of sugars in cell to cell recognition, blood groups.

OC(CB1)-2: Nucleic acids & lipids**15 Hrs**

Nucleic acids: Retro synthetic analysis of nucleic acids - Nucleotides, Nucleosides, Nucleotide bases and Sugars. Structure and synthesis of nucleosides and nucleotides. Primary, secondary and tertiary structure of DNA. Types of mRNA, tRNA and rRNA. Replication, transcription and translation. Genetic code. Protein biosynthesis. DNA finger printing.

Lipids: Introduction and classification of lipids. Stereochemical notation in lipids. Chemical synthesis and biosynthesis of phospholipids and glycolipids. Properties of lipid aggregates, micelles, bilayers, liposomes and biological membranes.

OC(CB1)-3: Proteins and Enzymes**15 Hrs**

Proteins: Introduction. Peptide bond, classification and nomenclature of peptides. Amino acid sequence of polypeptides and proteins: terminal residue analysis and partial hydrolysis. Peptide synthesis by solution phase and solid phase synthesis methods. Proteins - Biological importance and classification - Primary, secondary and tertiary structure of proteins.

Enzymes: Definition. Classification based on mode of action. Mechanism of enzyme catalysis - Lock and Key, Induced-Fit and three point contact models. Enzyme selectivity - chemo, regio, diastereo and enantio selectivity - illustration with suitable examples. Factors affecting enzyme catalysis. Enzyme inhibition - reversible and irreversible inhibition. Enzymes in organic synthesis. Immobilised enzymes

OC(CB1)-4: Coenzymes and Vitamins**15 Hrs**

Coenzymes: Introduction. Co-factors - cosubstrates - prosthetic groups.

Classification — Vitamin derived coenzymes and metabolite coenzymes. Structure and biological functions of coenzyme A, thiamine pyrophosphate (TPP), pyridoxal phosphate (PLP), oxidized and reduced forms of I) nicotinamide adenosine dinucleotide / their phosphates (NAD), NADH, NADP^+ NADPH) ii) Flavin adenine nucleotide FAD, FADH_2 and iii) Flavin mononucleotide (FMN, FMNH_2) lipoic acid, biotin, tetrahydrofolate and ubiquinone. Adenosine triphosphate (ATP) and adenosine diphosphate (ADP), S-adenosyl

methionine (SAM) and uridine diphosphosugars (UDP-sugars) Mechanism of reactions catalyzed by the above coenzymes.

Vitamins: Introduction, classification and biological importance of vitamins. Structure determination and synthesis of vitamins A, B₁, and B₂. Synthesis of vitamins - B₆, C, E and K. Structure of vitamin B₁₂.

Reference Books:

1. Organic Chemistry Vol.I and Vol.II by I.L.Finar
2. Carbohydrate Chemistry by Barton Volumes
3. Carbohydrate chemistry by G.J.Boons
4. The chemistry of natural products:vol.V - carbohydrates by S.F.Dyke
5. Organic Chemistry by McMurry
6. Nucleic acids in Chemistry and Biology by G M Blackburn MI Gait
7. Lehninger Principles of Biochemistry by D L Nelson and M MCoxon
8. Outlines of Biochemistry by Conn and Stumpf
9. Enzyme structure and mechanism by Fersht and Freeman
10. Enzymes for green organic synthesis by V.K.Ahluwalia
11. Biotransformations in Organic Chemistry by K Faber.
12. Principles of biochemistry by Horton & others.
13. Bioorganic chemistry - A chemical approach to enzyme action by Herman Dugas and Christopher Penney.
14. Concepts in Biotechnology by D.Balasubramanian & others
15. Chemistry and physiology of the vitamins by H.R.Rosenberg.

Paper-III CH (OC)303T (CB2): Forensic Chemistry & Toxicology

OC(CB2)-5: Forensic chemistry- I

OC(CB2)-6: Forensic chemistry- II

OC(CB2)-7: Forensic Toxicology-I

OC(CB2)-8: Forensic Toxicology-II

OC(CB2)-5: Forensic chemistry-I

15 Hrs

Forensic Chemistry - Introduction - Types of cases / exhibits - Preliminary screening - presumptive tests (colour and spot tests) - Examinations procedures involving standard methods and instrumental techniques

Qualitative and quantitative forensic analysis of inorganic and organic material - Chemical fertilizers (N,P,K) - Insecticides (Endosulfan, Malathion, Carbaryl) - Metallurgical analysis (Fe, Cu, Zn, Au, Ag) - Natural products (tobacco, tea, sugars, rubber) - Industrial chemicals - Sulphuric, Nitric and Hydrochloric acids, Sodium, Potassium hydroxide, Ammonium nitrate, Potassium chlorate, Organic solvents like Methanol, Ethanol, Acetone, Chloroform and Ether Organic chemicals like Acetanilide, P- Aminophenol, and Nitrobenzene etc. with reference to forensic work.

OC(CB2)-6: Forensic chemistry-II

15 Hrs

Examination of petroleum products - Distillation and fractionation - various fractions and their commercial uses - Standard method of analysis of petroleum products - Analysis of petroleum products for adulteration and arson residues. Chemistry of fire - Investigation and evaluation of fires - Causes of fire - Analysis of arson residues by conventional and instrumental methods. Analysis of trace evidence - Cosmetics, Dyes, Trap related evidence materials, Paints, Pigments, Fibres, Oils fats, Greases, Industrial dusts, Chemicals and Plant materials.

OC(CB2)-7: Forensic Toxicology-I

15 Hrs

Toxicology- Introduction- History- Scope- Areas of Toxicology- Role of forensic toxicologist- Poisons- Classification of poisons- Types of poisoning- Sample collection and preservation of toxicological exhibits in fatal and survival cases- Storage of samples- Signs and symptoms of poisoning- Toxicological investigation/examination of poisoned death- Interpretation of toxicological data- Courtroom testimony in toxicological cases. Case Histories.

OC(CB2)-8: Forensic Toxicology-II

15 Hrs

Principles of Toxicology- Introduction - Pharmacokinetics - Methods of transportation of toxicant- Absorption- Distribution- Storage of toxicants- Redistribution - Metabolism- Oxidation

- Reduction - Hydrolysis - Conjugation - Excretion- Other routes of elimination-Toxicokinetics-one and two compartmental model - Toxicodynamics- Spectrum of undesired(toxic) effects- Interaction of chemicals- Tolerance- Dose response relationship- Developmental and reproductive toxicity- Mutagenicity- Toxicity testing.

Recommended books:

1. James, S. H. and Nordby, J. J.: Forensic Science: An Introduction to Scientific and Investigative Techniques, 2003.
2. Saferstein, R: Criminalistics - An Introduction to Forensic Science, Prentice Hall, 1995.
3. Sarkar, S: Fuels and Combustion, Orient Longman, 1990
4. Verma, R. M: Analytical Chemistry – Theory and Practice, CBS Pub., 1994
5. Svehla, G. Ed.: Vogel's Qualitative Inorganic Analysis, Longman, 1998.
6. Bassett: Vogel's Text Book of Quantitative Inorganic Analysis, Longman, 1978
7. Vogel, A. I: Text Book of Practical Organic Chemistry including Qualitative Organic Analysis, ELBS, 1971.
8. Narayanan, T. V: Modern Techniques of Bomb Detection and Disposal, R. A. Security System, 1995.
9. Almirall, J. R. and Furton, K. G: Analysis and Interpretation of Fire Scene Evidence, CRC Press, 2004.
10. Bogusz, M. J: Handbook of Analytical Separations : Vol. 2 ,Forensic Science, Elsevier, 2000.
11. Bureau of Indian Standards: Specifications and Methods of Analysis for Petroleum Products.
12. Wilson and Wilson's Comprehensive Analytical Chemistry Volumes
13. Standard Methods of Chemical Analysis
14. AOAC: Official Methods of Analysis
15. Daeid, N.N.: Fire Investigation: Theory and Practice, Taylor and Francis, 2003
16. Klaassen, C. D.,: Casarett and Doull's Toxicology: The Basic Science of Poisons, 5th ed, McGraw-Hill, 1995.
17. Moffat, A.C. : Osselton, D. M. Widdop, B. : Clarke's Analysis of Drugs and Poisons in Pharmaceuticals, body fluids and postmortem material, 3rd ed., Pharmaceutical Press 2004.
18. Bogusz, M. J.,: Hand Book of Analytical Separations, Vol. 2: Forensic Science, 1st ed., Elsevier Science ,2000.
19. Siegel, J.A., Saukko, P. J., Knupfer, G.,: Encyclopedia of Forensic Sciences (Vol3), Academic Press, 2000.
20. Paranjape, H.M., Bothara, G.K., Jain, M.M.: Fundamentals of Pharmacology, 1st ed., Nirali Prakashan, 1990.
21. Budhiraja, R.D.: Elementary Pharmacology and Toxicology, Popular Prakashan, 2nd ed., 1999.
22. Laboratory procedure Manual, Forensic Toxicology: DFS, 2005
23. Cravey, R.H; Baselt, R.C.: Introduction to Forensic Toxicology , Biochemical Publications, Davis, C.A. (1981)
24. Stolmen, A.; Progress in Chemical Toxicology: Academic Press, New York (1963)
25. Modi, Jaisingh, P.; Textbook of Medical Jurisprudence & Toxicology, M.M. Tripathi Publication (2001)
26. Eckert; An Introduction to Forensic Science, CRC Press

Elective-4A

Paper-IV CH (OC) 304T (CB3): Green chemistry and Organic materials

OC (CB3) -9: Principles of Green chemistry

OC (CB3) -10: Green Synthesis

OC (CB3) -11: Organic nanomaterials

OC (CB3) -12: Supramolecular chemistry

OC (CB3)-9: Principles of Green Chemistry

15 Hrs

Green chemistry: Introduction

Principles of Green Chemistry: Designing a Green Synthesis using these principles; Prevention of Waste/by-products; maximum incorporation of the starting materials used in the synthesis into the final products (Atom Economy); prevention/minimization of hazardous/toxic products; designing safer chemicals; selection of appropriate auxiliary substances - green solvents, ionic liquids and solvent-free synthesis: energy requirements for reactions - use of microwaves, ultrasonic energy in organic synthesis; prevention of unnecessary derivatization – careful use of protecting groups; use of catalytic reagents in preference to stoichiometric reagents; designing of biodegradable products; prevention of chemical accidents; strengthening/development of analytical techniques to prevent and minimize the generation of hazardous substances in chemical processes.

OC (CB3) -10: Green Synthesis

15Hrs

i) Microwave Assisted Organic Synthesis (MAOS): introduction, benefits and limitations

a) Microwave assisted reactions in organic solvents: Esterification, Fries rearrangement, Claisen rearrangement and Diels- Alder reaction.

b) Microwave assisted Solvent-free reactions: Deacetylation, saponification of esters, alkylation of reactive methylene compounds and synthesis of nitriles from aldehydes.

ii) Ultrasound Assisted Organic Synthesis: introduction, applications of ultrasound- Cannizzaro reaction, Reformatsky reaction and Strecker synthesis.

iii) Organic Synthesis in Green Solvents: introduction

a) Aqueous Phase Reactions: Diels-Alder Reaction, Heck reaction, Hoffmann elimination, Claisen-Schmidt condensation hydrolysis and dihydroxylation reactions.

b) Organic Synthesis using Ionic liquids: Introduction, applications-Beckmann rearrangement Suzuki Cross-Coupling Reaction and Diels- Alder reaction.

iv) Green Catalysts in organic synthesis: introduction

a) Phase Transfer Catalysts in Organic Synthesis: Introduction, Williamson ether synthesis and Wittig reaction

b) Biocatalysts in Organic Synthesis: Biochemical (microbial) oxidations and reductions.

OC (CB3) -11: Organic Nanomaterials

15Hrs

Introduction: The 'top-down' approach, the 'bottom-up' approach and Nanomanipulation.

Molecular Devices: Photochemical devices, Liquid crystals, Molecular wires, Rectifiers, Molecular switches and Molecular Muscles.

New Carbon family: Types of Fullerenes, Types of Carbon nanotubes (Zig-Zag, Armchair and Chiral), Graphenes. Growth, Chemical Synthesis and optoelectronic properties of Fullerenes, CNTs (Zig Zag, Armchair and Chiral), singlewalled CNTs (SWCNTs) and multi walled MWCNTs) and Graphenes.

Structures of aromatics belts, nano car and molecular machines.

Optoelectronic molecules: OLEDs, Organic Solar Cells (Basic OLED mechanism and structures)

Natural Benzheterazoles and their synthetic modifications as optoelectronic molecules.

OC (CB3) -12: Supramolecular Chemistry

15Hrs

Introduction: Supramolecular interactions (ion-ion, ion-dipole, H-bonding, cation- π , anion- π , π - π and Van der Waals interactions), Ionophore and molecular receptors.

Host-Guest Chemistry: Lock and key analogy, Structures and applications of Cryptands, Spherands, Calixerenes, Cyclodextrins, Cyclophanes, Carcerands and hemicarcerands.

Self-assembly: Ladder, polygons, helices, rotaxanes, catenanes, Molecular necklace, dendrimers, self-assembly capsules their synthesis, properties and applications.

Enantioselective molecular recognition: Cyclodextrins, Crown ethers with chiral framework, Chiral receptor from Kemp's triacid. Chiral receptors for tartaric acid.

Recommended books:

1. P.T. Anastas & J.K. Warner: Oxford Green Chemistry- Theory and Practical, University Press (1998).
2. A.S. Matlack: Introduction to Green Chemistry, Marcel Dekker, (2001).
3. M.C. Cann & M.E. Connely: Real-World cases in Green Chemistry, American Chemical Society, Washington (2000).
4. M.A. Ryan & M. Tinnesand, Introduction to Green Chemistry, American Chemical Society, Washington (2002).
5. V.K. Ahluwalia & M.R. Kidwai: New Trends in Green Chemistry, Anamalaya Publishers
6. Enantioselective organocatalysis, Peter I. Dalko, Wiley-VCH
7. Core Concepts in Supramolecular Chemistry and Nanochemistry by Jonathan W. Steed, David R. Turner and Karl J. Wallace; John-Wiley and Sons Publications
9. Supramolecular Chemistry by Jonathan W. Steed and Jerry L. Atwood, John-Wiley and Sons Publications
10. Supramolecular Chemistry-Concepts and Perspectives by J.M. Lehn; Wiley-VCH (1995) Publications
11. Supramolecular Chemistry by P. D. Beer, P. A. Gale and D. K. Smith; Oxford University Press (1999)
12. Stereochemistry of organic compounds -Principles & Applications by D. Nasipuri
13. Nanochemistry by G.B. Sergeev; Elsevier
14. Nanochemistry: A chemical approach to nano materials, G.A. Ozin & A.C. Arsenault; RSC publishers.

Elective-4B

Paper-IV CH (OC) 304T (CB4): Pesticides

OC(CB4)- 13:Introduction to pesticides

OC(CB4)- 14: Synthetic insecticides

OC(CB4)- 15:Natural insecticides& herbicides

OC(CB4)- 16:Fungicides, and Rodenticides

OC (CB4)-13: Introduction to pesticides

15 Hrs

i) **Defination** ,Classification and importance of pesticides

ii) **Pest control**: Different methods –chemical – insecticides, fungicides, herbicides, rodenticides, fumigants, chitin synthesis inhibitors and insect repellents.

a) **Biological**–pheromones: Definition and classification, synthesis of Disparlure, Exobrevicomin, Endobrevicomin, frontalin and grandiso pheromones, synthetic sex attractants.

b) Insect juvenile hormones: JH-A, JH-B,Synthesis of juvabione. Structural formula and importance of methopren.

c) Moultingharmones-structural formulae and mode of action of ecdysones

d) Antibiotics and secondary metabolites of microbial origin as insecticides and fungicides in agricultiure. Structural formula and importance of Blastacidin-S, Kasugamycin, Avermectin-B, Invermectin, piercidins and phytoalexins.

iii) **Environmental pollution from pesticides**.iv) Integrated pest management.

v) Pesticide formulations: Dusts, Granules, Wettable powders, Emmulsions and Aerosols.

OC (CB4)- 14: Synthetic insecticides

15 Hrs

i)**Organochlorine insecticides**- synthesis and mode of action of methoxychlor, perthan, Dicofol, Heptachlor, Dieldrin and Endosulfan.

ii) **Organophosphorous insecticides** –synthesis and mode action of Phosphoric acid derivatives, phosdrin, Dichlorophos, parathion, Zolone, Aninphomethyl, TEPP and Sachradan.

iii) **Carbamate insecticides**- synthesis and mode of action of carbamyl, Furadan, Baygon, Aldicarb and Zectron.

iv) Formulation and residue analysis of organochlorine, organophosphorous and carbamate insecticides.

OC (CB4)- 15: Natural insecticidesand herbicides15 Hrs

i) **Insecticides of palnt origin** –synthesis and importance of pyrethrins (I and II), Rotenone and Nicotine. Main constituents Neem-structural formula of Azadirachtin. Synthesis of polygodial and warbunganol(Antifeedants).

ii)Synthesis of pyrethroids: synthesis of Allethrin, Bioallethrin, Cypermethrin, Fenvalerate, Decemethrin and pyrithrelone.

iii) **Concept of Bioinsecticides** – Bacillus thiuringiensis.

iv) **Concept of pro-insecticides**-structure and mode of action of pro-pheromones and pre-pro-insecticides.

v) **Herbicides** – synthesis,applications and mode of action of the following

a)Aryloxyalkyl carboxylic acid derivative:2,4-D, MCPA,2,4,5-T and 2,4,5-TP.b) Carbamates-propham and chloropham, c)Urea derivatives –Monouron and diuron, d) Aliphatic acids-Dalapon,TCA, e)Aromatic acids -2,3,6-TBA,Dicomba and Amiben, f)Nitrogen heterocyclic dericvatives –Simazine,Atrazine,Amitrole,Maleic hydrazide Diquat and paraquat, g) Phenols-PCP and Dinoseb, h) Benzonitrile compounds

OC (CB4)-16: Fungicides, and Rodenticides**15 Hrs****i) Fungicides** –classification ,synthesis application and mode of action of the following classes:**a)**Carbamates**b)**Quinones-chloranil,Dichloneand Benquinox**c)**perchloromethylmercaptan derivative –captan,folpet,Difolatan and Mesulfan **d)** Benzimidazoles-carbendazim, Benomyl and Thiabendazole**ii) Rodenticides**, **a)** Anticoagulents-synthesis and application of warfarin, Coumachlor, Vacor, Coumatetrallyl, Dicoumarol and Bromodiolen.**b)** Acute poisons- application of pindone,Ratindan,SodiumFluoroacetate ,Barium fluoroacetate,Antu,Tetramine,pindone and castrix.**Referencebooks:**

- 1) Naturally occurring insecticides: M.Jacobson and D.G.Crosby.
- 2) Insecticides for future:Jacobson
- 3) Insect juvenile hormone chemistry and action : J.J Mann and M.Beroza
- 4) Polygodial and warburganal.Terpenoidantifeedants part-II rec,Tran,chin 106
- 5) Insect antifeedants :S.V.ley&P.L Toogood,chemistry in Britain ,Jan 1990 P.31
- 6) Synthesis of Insecticides :Metcalf
- 7) Fungicides-Frear
- 8) Fungicides-Nene
- 9) Residue reviews vol.36 : Melnikov
- 10) Safer insecticides :E.Hodgson
- 11) Crop protection agents from Nature: leonard G Copping
- 12) Biofertilizers and Bioinsecticides : A.M.Deshmukh
- 13) Insecticides and Fungicides :U Sriramulu.
- 14) Organo chlorine insecticides : persistent organic pollutants :F.Moriary
- 15) Herbicides :P.C.Kearney&D.D.Kaufnan
- 16) Analytical Method for pesticides :Z.Weig (Vol III)
- 17) Pesticide formulations :Van Valkenburg
- 18) Insecticides :A.S.Tahori
- 19) Herbicides,fungicides,formulation chemistry-A.S.Tahori
- 20) Environmental pollution by pesticides :C.A.Edwards
- 21) Pespticides managements and insecticide resistance :Watson and brown
- 22) Organo phosphorous pesticides M.eto

Laboratory courses:

Paper CH (O) 351P: Synthesis of organic molecules, isolation of natural products & TLC

(A) Laboratory synthesis of the following compounds:

2-Phenyl indole (Fischer indole synthesis), 7-hydroxy-3-methyl flavone (Baker-Venkatraman reaction), 2,5-Dihydroxy acetophenone (Fries reaction), 4- Chlorotoluene from p-toluidine (Sandmeyer reaction), Benzilic acid from benzoin (Benzilic acid rearrangement), Benzpinacol (photochemical reaction), 7-hydroxy coumarin (Pechman synthesis), Photo-dimerization of maleic anhydride, benzophenone (Friedel-Crafts reaction), Benzanilide (Beckmann rearrangement), Vanillyl alcohol from vanillin (NaBH_4 reduction), 2- and 4-nitrophenols (nitration and separation by steam distillation), Acridone from Phthalic anhydride.

(B) Isolation of the following natural products:

Caffeine from tea leaves (solvent extraction), Piperine from pepper (Soxhlet extraction), Eucalyptus oil from leaves (steam distillation), Lycopene from tomatoes.

(C) Thin layer chromatography : Thin layer chromatography: Determination of purity(All the above preparations) , monitoring the progress of chemical reactions (any of the four above preparations), identification of unknown organic compounds by comparing the R_f values of known standards.

Paper CH (O) 352P: Separation and identification of organic compounds & Column chromatography

Separation of two component mixtures by chemical methods and their identification by chemical reactions — separation by using solvent ether, 5 % aqueous sodium bicarbonate, 5% sodium hydroxide and dil hydrochloric acid, checking the purity of the two components by TLC, identification of the compounds by a systematic study of the physical characteristics (mp/bp), extra elements (nitrogen, halogens and sulfur), solubility, functional groups, preparation of crystalline derivatives and identification by referring to literature. A minimum of 09 mixtures should be separated and analyzed by these procedures.

Cannizzaro reaction: 4-Chloro benzaldehyde as substrate and separation of the resulting two component mixture

Separation of three component mixtures by chemical methods. A minimum of two mixtures should be separated and analyzed.

Column chromatography: Separation of a mixture of *ortho* and *para*-nitroanilines and any one of the two component mixture using silica gel as adsorbent and chloroform as the eluent. The column chromatography should be monitored by TLC.

Recommended Books:

1. Practical organic chemistry by Mann & Saunders
2. Text book of practical organic chemistry by Vogel
3. The systematic identification of organic compounds by Ralph L. Shriner, Christine K. F. Hermann, Terence C. Morrill and David Y. Curtin

M.Sc. ORGANIC CHEMISTRY SPECIALISATION

IV SEMESTER SYLLABUS

(For the batch admitted during the academic year 2016-2017)

Paper-1 CH (OC) 401T: Drug Design and Drug Discovery

OC-17: Principles of Drug design and drug discovery

OC-18: Lead modification and SAR Studies

OC 19: QSAR studies and computer aided drug design

OC-20: Combinatorial Synthesis

Paper-II CH (OC) 402T: Drug synthesis and mechanism of action

OC-21: Drugs acting on metabolic process, cell wall and specific enzymes

OC-22: Drugs acting on genetic material and immune system

OC-23: Drugs acting on receptors and ion channels

OC-24: Chiral drugs

Elective-3A Paper-III CH (OC)-403T (CB1): Advanced Heterocyclic Chemistry

OC (CB1) 17: Non aromatic heterocyclics & aromaticity

OC (CB1) 18: Five and six membered heterocyclics with two hetero atoms

OC (CB1) 19: Heterocyclics with more than two hetero atoms

OC (CB1) 20: Larger ring and other heterocycles

Elective-3B Paper-III CH (OC)-403T (CB2): Polymers, dyes and Pigments

OC (CB2) 21: Polymers- I

OC (CB2) 22: Polymers- II

OC (CB2) 23: Dyes-I

OC (CB2) 24: Dyes-II and pigments

Elective-4A Paper-IV CH (OC) 404(CB3)T: Advanced Natural Products

OC(CB3)-25: Biosynthesis of natural products

OC(CB3)-26: Structure determination of natural products -I

OC(CB3)-27: Structure determination of natural products-II

OC(CB3)-28: Total stereo selective synthesis of natural products.

Elective-4B Paper-IV CH (OC) 404(CB4)T: Biopharmaceutics and Pharmacodynamics

OC(CB4)-29 : Pharmacokinetics

OC(CB4)-30 : Pharmacodynamics

OC(CB4)-31 : Principles of Therapeutics

OC(CB4)-32: Drug Interactions

Laboratory courses

Paper-VCH (OC) 451P: Spectroscopic identification of organic compounds & practice of chemistry software programmes

Paper-VI CH (OC) 452P: Synthesis and analysis of drugs

M.Sc. CHEMISTRY (ORGANIC CHEMISTRY)

IV SEMESTER SYLLABUS

(For the batch admitted during the academic year 2016 -2017 under the CBCS pattern)

Paper-1 CH(OC) 401T: Drug Design and Drug Discovery

OC-17: Principles of Drug design and drug discovery

OC-18: Lead modification and SAR Studies

OC 19: QSAR studies and computer aided drug design

OC 20: Combinatorial Synthesis

OC- 17: Principles of Drug design and drug discovery 15 Hrs

Introduction to drug discovery. Folklore drugs, stages involved in drug discovery- disease, drug targets, bioassay. Discovery of a lead- screening of natural products and synthetic compound libraries. Existing drugs as leads (me too drugs). Pharmacokinetics (ADME), pharmacodynamics. Nature of drug – receptor interactions and their theories – Occupancy theory, Induced – fit theory, Macromolecular perturbation theory and Two-state model of receptor activation. Natural products as lead structures in drug discovery – Pharmacophore - structure pruning technique e.g. morphine. Discovery of lead structure from natural hormones and neurotransmitters. Principles of design of agonists (e.g. Salbutamol), antagonists e.g. cimetidine) and enzyme inhibitors (e.g. captopril). Drug discovery without lead – serendipity- Penicillin and Librium as examples. Principles of prodrug design. Introduction to drug patents and Clinical trials.

OC-18: Lead modification and SAR Studies 15 Hrs

SAR: Lead modification strategies, Bioisosterism, variation of alkyl substituents, chain homologation and branching, variation of aromatic substituents, extension of structure, ring expansion and ring contraction, ring variation, variation and position of hetero atoms, ring fusion, simplification of the lead, rigidification of lead. Discovery of oxamiquine, salbutamol, cimetidine and captopril. Structure-Activity Relationship studies in sulfa drugs, benzodiazepines, and taxol analogs.

OC-19: QSAR studies and computer aided drug design 15Hrs

QSAR: Introduction, physicochemical properties - pK_a , electronic effects and Hammett constants (σ), lipophilicity constant (π), steric effects and Taft's constant, linear and nonlinear relationship between biological activity. Lipophilicity Substituent constants. Lipinski rule of five. Hansch analysis, Craig's plot, Topliss scheme, Free Wilson approach, cluster significant analysis. Two case studies (QSAR study on pyranamine and design of Crizotinib).

Computer aided drug design: Introduction, active site, allosteric binding site, use of grids in docking, rigid docking, flexible docking and induced fit docking of ligands. Basic principles and difference between structure and ligand based drug design, de novo drug design and utility to optimize the lead structure.

OC-20: Combinatorial Synthesis**15Hrs**

Introduction. Combinatorial approach. Combinatorial libraries, technologies. Solid phase synthesis, types of resins. Linkers. Reactants for solid phased synthesis. Methods of Parallel synthesis: Haughton's tea bag procedure. Automated parallel synthesis. Methods in Mixed combinatorial synthesis: general principles. Furkas mix and split combinatorial synthesis, Structure determination of active compounds-Deconvolution, Methods in deconvolution-recursive deconvolution, tagging and use of decoded sheets. Examples of Combinatorial Chemistry. Planning and designing of combinatorial synthesis, Spider like scaffolds, drug molecules. Automation in Combinatorial chemistry. High throughput screening.

Reference books

1. Burger's medicinal chemistry and drug discovery by Manfred E. Wolf.
2. Introduction to Medicinal chemistry by Patrick.
3. Introduction to drug design by R Silverman
4. Comprehensive medicinal chemistry. Vol 1-5 by Hanzsch.
5. Principles of medicinal chemistry. by William Foye
6. Biochemical approach to medicinal chemistry. by Thomas Nogrady.
7. Pharmaceutical Chemistry and Drug synthesis by Roth and Kleeman
8. Drug design by E.J.Arienes
9. Principles of Medicinal Chemistty Vol I & II by Kadam et al
10. Medicinal chemistry An introduction by Garreth Thomas
11. Organic and Pharmaceutical chemistry By Delgrado
12. Organic Pharmaceutical chemistry By Harikishansingh
13. Medicinal Chemistry By Ashtoshkar
14. Medicinal Chemistry By Chatwal
15. Organic Drug synthesis By Ledneicer Vol 1-6
16. Strategies for organic drug synthesis and design By Daniel Ledneicer.
17. Top Drugs: Top synthetic routes By John Saunders
18. Chirotechnology By Roger A. Sheldon
19. Burger's Medicinal Chemistry and Drug Discovery: Principles and Practices. Vol. 1.
20. Medicinal Chemistry by G. Patricks.
21. Text book of Drug Design and Discovery, Edited by PovlKrogsgaard – Larsen Tommy Liljefors.
22. Structure Based Drug Design of Crizotinib (PF-02341066), a Potent and Selective Dual Inhibitor of Mesenchymal–Epithelial Transition Factor (c-MET) Kinase and Anaplastic Lymphoma Kinase (ALK) Martin P. Edwards, J. Med. Chem., 2011, 54 (18), pp 6342–6363.
http://www.pfizer.com/news/featured_stories/featured_stories_martin_edwards.jsp

Paper-II CH (OC) 402T: Drug synthesis and mechanism of action

OC-21: Drugs acting on metabolic process, cell wall and specific enzymes

OC-22: Drugs acting on genetic material and immune system

OC-23: Drugs acting on receptors and ion channels

OC-24: Chiral drugs

OC-21: Drugs acting on metabolic process, cell wall and specific enzymes

Basic concepts of mechanism of drug action: Introduction to macromolecular targets, carbohydrates, proteins, lipids and nucleic acids as possible drug targets. Classification of drugs. Enzyme inhibition and its types.

a) Drugs acting on metabolic process:

Antifolates –Discovery and mechanism of action of sulphonamides, Synthesis of sulfomethoxazole, sulfadoxine, sulfaguanidine and dapsone.

Diaminopyrimidines -trimethoprim, bacterial resistance to sulfonamides and drug synergism

b)Drugs acting on cell wall: Structure of bacterial cell wall, β -Lactam antibiotics – mechanism of action of penicillins and cephalosporins. Synthesis of penicillin-G and cephalosporin-C, cefalexin and cycloserine. Resistance to penicillins, broad spectrum penicillins – cloxacillin, methicillin, ampicillin, amoxicillin and carbenicillin. β -Lactamase inhibitors- Structural formulae and mode of action of clavulanic acid and sulbactam

c)Drugs acting on specific enzymes: H^+/K^+ -ATPase inhibitors- synthesis of Omeprazole and Carbonic anhydrase inhibitors-synthesis of Acetazolamide.

OC-22: Drugs acting on genetic material and immune system

Drugs acting on genetic material:Introduction, classification and mechanism of action.

a) DNA-intercalating agents-Anticancer and antimalarial agents. Structural formulae of Daunomycin, Adriamycin and Amsacrine. Synthesis of Amsacrine, Nitracrine, Quinacrine and Chloroquine.

b) DNA- Binding and nicking agents: Antiprotozoal drugs. Synthesis of Metronidazole, Dimetridazole and Tinidazole.

c) DNA-Alkylators: Synthesis of Cyclophosphamide and Bisulphan.

d) DNA-Polymerase inhibitors: Antiviral agents- Synthesis of Acyclovir and AZT.

e) DNA-Topoisomerase inhibitors: Anti bacterial agents.Synthesis of Ciprofloxacin and Norfloxacin. Structural formulae ofloxacin and Lomefloxacin.

f) Inhibitors of transcribing enzymes: Anti-TB and antileprosy agents-structural formulae of Rifamycins and partial synthesis of Rifampicin.

g) Drugs interfering with translation process: Antibacterial drugs- Structural formulae of Erythromycin, 5-Oxytetracycline and Streptomycin. Synthesis of Chloromycetin

Drugs acting on immune system: Introduction to immune system. Immunosuppressing agent-structural formula of Cyclosporin. Immunoenhancers-use of vaccines and structural formula of levamisole.

OC-23: Drugs acting on receptors and ion channels

Introduction to nervous system: structure of neuron, nerve transmission. Definition and examples of agonist, antagonist, neurotransmitters and receptors.

Drugs acting on receptors:

a)Adrenergic receptors - Introduction and classification. α -Adrenergic-receptor agonists and antagonists- Synthesis and biological activity of Nor-adrenaline, Methyl L dopa and Tetraizosin.

β-Adrenergic-receptor - agonists and antagonists – Synthesis and pharmacological activity of Salbutamol, Terbutaline, Propranolol and Atenolol.

b)Cholinergic-receptors: Introduction and classification.Cholinergic-receptor agonists and antagonists- Structural formulae of Nicotine, Atropine and Tubocurarine. Synthesis of Acetylcholine and Succinylcholine

c)Dopamine receptors: Introduction and classification.Dopamine- receptoragonists and antagonists- Biosynthesis of Dopamine. Synthesis of L-Dopa and Chlorpromazine.

d)Serotonin receptors: Introduction and classification.Serotonin receptoragonists and antagonists-synthesis and pharmacological activity of Serotonin and Metoclopramide.

e)Histamine receptors:Introduction and classification.Histamine receptor agonists and antagonists-synthesis and biological action of Histamine, Chlorpheniramine, and Ranitidine.

f) Hormones and their receptors: Introduction to estrogen receptors, Structural formulae of Tamoxifen

Drugs acting on ion channels: Introduction to ion channels, drugs acting on Ca^{2+} , Na^{+} and Cl^{-} channels and their mode of action. Structural formulae of Tetracaine and synthesis and of Nifedipine, Diltiazem, Tetracaine and 4-Aminopyridine.

OC-24: Chiral drugs

Introduction to chiral drugs. Three-point contact model, Eutomer, Distomer and eudesmic ratio. Pfeiffer's rule. Role of chirality on biological activity: Distomers – a) with no side effects b)with undesirable side effects c) both isomers having independent therapeutic value d)combination products having therapeutic advantages e) metabolic chirality inversion.

Synthesis and pharmacological activity of S-Ibuprofen, S- Metoprolol, Ininavir sulfate, Levocetazine, 2S-Verapamil, S,S-Ethambutol, (+)Lomefloxacin, Fluvastatin, Dextropropoxyphen, (+)Ephedrine, (+)Griseofulvin, Dexormaplatin, R-Indacrinone, Nateglinide, Oxybutynin hydrochloride, S,S- Captopril and S,S,S- Enalaprilate.

Reference Books:

1. Burger's medicinal chemistry and drug discovery. By Manfred B. Wolf.
2. Introduction to Medicinal chemistry. By Graham Patrick.
3. Introduction to drug design. By R.B.Silverman
4. Comprehensive medicinal chemistry. Vol 1-5 by Hanzsch.
5. Principles of medicinal chemistry. By William O. Foyeetal.
6. Biochemical approach to medicinal chemistry. By Thomas Nogrady.
7. Pharmaceutical Chemistry and Drug synthesis By Roth and Kleeman
8. Drug design By E.J. Arienes
9. Principles of Medicinal Chemistry. Vols.1 & 2 By Kadam etal
10. Medicinal chemistry An introduction By Gareth Thomas
11. Wilson and Gisvold,s text book of Organic, Medicinal and Pharmaceutical chemistry By J.N.Delgado and W.A.Remers.
12. Organic Pharmaceutical chemistry By Harikishansingh.
13. Medicinal Chemistry By Ashutoshkar
14. Medicinal Chemistry By G.Chatwal
15. Organic Drug synthesis By Ledneiser Vol 1-6
16. Strategies for organic drug synthesis and design By Daniel Ledneiser
17. Top Drugs: Top synthetic routes By John Saunders
18. Chirotechnology By Roger A. Sheldon

Elective-3A

Paper-III CH (OC)-403T (CB1): Advanced Heterocyclic Chemistry

OC (CB1) 17: Non aromatic heterocyclics& aromaticity

OC (CB1) 18: Five and six membered heterocyclics with two hetero atoms

OC (CB1) 19: Heterocyclics with more than two hetero atoms

OC (CB1) 20: Larger ring and other heterocycles

OC (CB1) 17: Nonaromatic heterocyclics& Aromaticity 15 Hrs

Different types of strains, interactions and conformational aspects of nonaromatic heterocycles. Synthesis, reactivity and importance of the following ring systems. Azirines, Aziridines, Oxiranes, Thiiranes, Diazirenes, Diaziridines, Oxaziridines, Azetidines, Oxetanes and thietanes

Aromaticity: Introduction, Aromatic and anti aromatic compounds. Criteria for aromaticity. Huckel's $4n+2$ electron rule for benzene and non benzenoid aromatic compounds. Eg. Cyclopropenium ion, cyclopentadienyl ion, cycloheptatrienium ion, azulene and annulenes.

OC (CB1) 18: Five and six membered heterocyclics with two hetero atoms 15 Hrs

Synthesis, reactivity, aromatic character and importance of the following heterocycles: Pyrazole, Imidazole, Oxazole, Thiazole, Isoxazole, Isothiazole, Pyridazine, Pyrimidine. Pyrazine, Oxazine, thiazine, benzimidazole, benzoxazole and benzthiazole.

OC (CB1) 19: Heterocyclics with more than two hetero atoms 15 Hrs

Synthesis, reactivity, aromatic character and importance of the following Heterocycles: 1,2,3-triazoles, 1,2,4-triazoles, Tetrazoles, 1,2,4-oxadiazole, 1,3,4-oxadiazole, 1,2,5-oxadiazole, 1,2,3-thiadiazoles, 1,3,4-thiadiazoles, 1,2,5-thiadiazoles, 1,2,3-triazine, 1,2,4-triazine, 1,3,5-triazine, tetrazines. Synthesis and importance of purines and pteridines. Synthesis of Caffeine, theobromine and theophylline.

OC (CB1) 20: Larger ring and other Heterocycles 15 Hrs

Synthesis, structure, stability and reactivity of Azepines, Oxepines and Thiepinines. Synthesis of Diazepines rearrangements of 1,2-diazepines. Synthesis of Benzoazepines, Benzodiazepines, Benzooxepines, Benzothiepinines, Azocines and Azonines. Synthesis of selenophenes, Tellerophenes, Phospholes and Boroles.

Recommended Books:

1. Heterocyclic Chemistry, T.Gilchrist
2. An introduction to the Chemistry of heterocyclic compounds, R.M.Acheson
3. Heterocyclic Chemistry, J.A.Joule&K.Mills
4. Principles of Modern Heterocyclic Chemistry, A.Paquette
5. Heterocyclic Chemistry, J.A.Joule& Smith
6. Handbook of Heterocyclic Chemistry, A.R.Katritzky
7. The aromaticity III level, units 17-19 British open university volumes
8. Aromatic character and aromaticity by G.M.Badger
9. Non-benzenoid aromatic compounds by D.Ginsberg
10. Nonbenzenoid compounds by Lloy

Elective-3B

Paper-III CH (OC)-403T (CB2): Organic Polymers, Dyes and Pigments

OC (CB2) 21: Polymers- I

OC (CB2) 22: Polymers- II

OC (CB2) 23: Dyes-I

OC (CB2) 24: Dyes-II and pigments

OC (CB2) 21: Organic Polymers - I 15 Hrs

Introduction, Classification of Polymers – according to origin, structure, intermolecular interactions. Types of polymerization – addition, condensation, radical, ionic and copolymerization with mechanism, Ziegler-Natta polymerization with mechanism. Stereochemistry of polymers, Plasticity – types of plastics. Molecular mass of polymers. Resins and plastics – Polystyrene and styrene copolymers, poly(vinyl chloride/vinyl acetate) and related polymers, acrylic polymers, polyesters, phenol-formaldehyde polymers, polyurethanes and epoxide polymers with examples. Natural and synthetic rubbers.

OC (CB2) 22: Organic Polymers - II

15 Hrs

a) Functional polymers :

i) Electrically conducting polymers: Introduction, basic principles. Brief description of polyanilines, polypyrroles, polyacetylenes, polythiophenes and their applications.

ii) Photoconductive polymers: Liquid crystal polymers, smectic, nematic and cholesteric structures, ion-exchange polymers – cationic, anionic exchange polymers and their uses.

iii) Smart materials: Uses in sensing device and communication networks.

iv) Biodegradable polymers: Definition, classification. Brief description polyhydroxyalkanoates, polycaprolactones, polylactic, polyvinyl alcohol and their applications.

b) Membranes: Filtration, micro, ultra, nano filtration. Separation of gases-Permeability and gas permeability representative polymers. Liquid separation-dialysis, electroosmosis and reverse osmosis.

c) Fire retarding polymers and photonic polymers.

Polymers in biomedical application, artificial organs and controlled drug delivery.

OC (CB2) 23: Dyes – I

15 Hrs

Synthetic and Natural dyes

Introduction, nomenclature and classification of synthetic dyes. Color and constitution - chromophores and auxochromes with suitable examples, Witt's theory, Armstrong's theory, Baeyer's theory, Nietzki's theory, Waston's theory, Modern theories, Valence Bond Theory and Molecular orbital theory. Chemistry and synthesis of triphenyl methane dyes [malachite green, rosaniline, para aniline blue, crystal violet methyl violet, hydroxytriphenyl methane dyes, Aurin, chrome violet], Azo dyes - types of azo dyes, synthesis of acidic and basic azo dyes, mono azo, di azo, tri azo and poly azo dyes. Chemistry and synthesis of cyanine dyes. Natural dyes – structure determination and synthesis of alizarine, Quinazarin and Indigo.

OC (CB2) 24: Dyes-II and Pigments

15 Hrs

a) Introduction to Fluorescence dyes

Interaction of organic molecules with electromagnetic radiation. Energy diagram. Activation and deactivation of organic molecules by light. Fluorescence and delayed fluorescence. Effect of molecular structure on fluorescence. General properties of fluorescent dyes and their requirements. Triplet-triplet absorption of organic molecules. Fluorescent quantum

yields and factors affecting them. Synthesis of Fluorescent aromatic hydrocarbons. and Fluorescent heteroaromatic compounds.

b) **Introduction to laser dyes.** Synthesis of Oligophenylenes. Oxazoles and benzoxazoles. Stilbenoid compounds Coumarin laser dyes, Rhodamine laser dyes.

c) **Pigments:** Introduction, Structures of Porphyrins, Bile pigments. Synthesis of Haemin and Chlorophyll. Synthetic pigments – preparation of phthalocyanines.

Reference Books

1. Organic polymer chemistry by K.J. Sanders
2. Polymer syntheses, Vol. I by S.R. Sandler and W. Karo
3. The elements of Polymer Science and Engineering by A. Rudin
4. Principles of Polymer Chemistry by A. Ravve
5. Polymer Science by V.R. Gowariker, N.V. Viswanathan and J. Sreedhar
6. Polymer Chemistry by C.E. Carraher, Jr.
7. A text book of polymers, Vol. I, II, III, M.S. Bhatnagar, S. Chand
8. Polymer Chemistry, B. Vollmert
9. Textbook of Polymer Science, F. W. Billmeyer Jr, John Wiley & sons
10. Organic Chemistry, Vol. 1, 2 by I.L. Finar
11. Color and constitution of organic molecules by J. Griffiths
12. Functional Dyes, Elsevier BV 2006, S.H. KIM
13. Colorants for non-textile Applications, Elsevier BV 2000 ... H.S. Freeman and A.T. Peters
14. Industrial Dyes-Chemistry, Properties, Applications. WILEY-VCH Verlag, 2003
Klaus Hunger
15. Introduction to Fluorescence Sensing, Springer 2009, by A.P. Demchenko
16. Natural Dyes and their Applications in Textiles by M. L. Gulrajani, IIT Delhi
17. Handbook on Natural Dyes for Industrial Applications by P. S. Vankar, National Institute of Industrial Research
18. Stereoelectronic Effects in Organic Chemistry by Pierre Deslongchamps, Pergamon Press
19. Chemistry and Biochemistry of plant pigments, Vol. 2, by T.W. Goodwin
20. Contemporary Polymer Chemistry, H. R. Alcock & F. W. Lambe, Prentice Hall
21. Materials science and engineering an introduction by William D Callister, Jr. Wiley Publishers

Elective-4A(ID Paper)

Paper-IVCH (OC) 404(CB3)T: Advanced Natural Products

OC(CB3)-25: Biosynthesis of natural products

OC(CB3)-26: Structure determination of natural products-I

OC(CB3)-27: Structure determination of natural products-II

OC(CB3)-28: Total stereo selective synthesis of natural products.

OC(CB3)-25: Biosynthesis of natural products 15 Hrs

Biosynthesis of secondary metabolites: Introduction, Difference between Laboratory synthesis and biosynthesis. Methods for determination of biosynthetic mechanism. Isolation and identification of Biosynthetic precursors, Feeding experiments – use of radioisotopes Measurement of incorporation – absolute incorporation, specific incorporation. Identification of the position of labels in labeled natural products by chemical degradation and spectral methods. Major biosynthetic pathways: 1) Acetate-Malonate pathway: Biosynthesis of aromatic compounds, 2) Shikimic acid pathway ; Biosynthesis of essential amino acids – phenylalanine, tyrosine and tryptophan, carboxylic acid derivatives, flavonoids and morphine alkaloids. 3) Mevalonic acid pathway : Biosynthesis of terpenes – mono, sesqui, di, tri (β -amyrin) and carotenoids, steroids – cholesterol.

OC(CB3)-26: Structure determination of natural products-I 15 Hrs

Determination of structure and stereochemistry of morphine, reserpine, abietic acid, cholesterol and rotenone.

OC(CB3)-27: Structure determination of natural products-II 15 Hrs

Spectroscopic techniques IR, UV, ^1H nmr, ^{13}C nmr, COSY, HETEROCOSY, NOESY, 2D-INADEQUATE and MS in the structure elucidations of natural products, Examples, flavones, biflavones, flavanones, isoflavones, coumarins, quinolines, isoquinolines.

Study of the following solved problems: Mass, IR, ^1H , ^{13}C NMR, HOMOCOSY, HECTOR, DEPT, 2D-INADEQUATE and NOE of Geraniol, INEPT of **menthol**, APT of **apiparine**,

Heteronuclear 2D-J resolved spectrum of **stricticine**, NOESY of **buxaquamarine**, HETEROCOSY of **strictanol**, 2D-INADEQUATE of **α -picoline** and **β -methyl tetrahydan furan**.

OC(CB3)-28: Total stereoselective synthesis of natural products. 15 Hrs

Nicalou's synthesis of Dynemicin A , Corey's synthesis of prostaglandins (E2, F2 α) and paeoriflorin, Sharpless synthesis of L-hexoses, Nicolaous synthesis of taxol, Danishefsky synthesis of indolizomycin, Takasago synthesis of menthol, Hoffmann-LaRoche synthesis of Biotin.

Reference books:

1. Textbook of organic chemistry, Vol II by I L Finar
2. Chemistry of natural products, Vol 12, by Atta-Ur-Rahman
3. An introduction to the chemistry of terpenoids and steroids, by William templeton
4. Systematic identification of flavonoid compounds by Mabry & Markham
5. Steroids by Fieser and Fieser
6. Alkaloids by Manske
7. Alkaloids by Bentley
8. The chemistry of terpenes by A Pinder
9. The terpenes by Simenson
10. Terpenoids by Mayo
11. Alkaloids by Pelletier
12. Total synthesis of Natural Products by Apsimon Vol 1-5
13. Biosynthesis by Geismann
14. Principles of organic synthesis 3rd Ed. R O C Norman and J M Coxen
15. One and two dimensional nmr spectroscopy by Atta Ur Rahman
16. Classics in total synthesis K C Nicolaou and E J Sorenson
17. Spectrometric identification of organic compounds by Silverstein and Webster

Elective-4B(ID Paper)

Paper-IV CH (OC) 404(CB4)T: Biopharmaceutics and Pharmacodynamics

OC(CB4)-29 : Pharmacokinetics

OC(CB4)-30 : Pharmacodynamics

OC(CB4)-31 : Principles of Therapeutics

OC(CB4)-32: Drug Interactions

OC(CB4)-29: Pharmacokinetics.

Introduction and importance of ADME studies of drugs. Routes of administration .
i)Absorption: Definition, absorption of drugs across the membranes. Physico chemical factors affecting the drug absorption (emphasis on pH partition hypothesis and Drug Dissolution). Methods of determination of drug absorption. Bioavailability. ii)Distribution: Apparent volume of drug distribution. Factors affecting distribution, plasma protein binding. iii) Metabolism: Sites of drug metabolism, metabolic rate constant, bioactivation and biotransformation of drugs (phase I and phase II reactions) iv)Elimination: Types of elimination and overall apparent elimination rate constant and half-life, concept of clearance.

OC(CB4)-29: Pharmacodynamics.

Introduction, targets for drug action, receptor concept. Pharmacological binding terms. Two-statereceptor model, receptor families- structure and signal transduction mechanisms- channel linked proteins, gating mechanism, G-protein coupled receptors, G-protein and their role, Targets for G-proteins, Kinase linked receptors, receptors that regulate gene transcription. Theories of concentration -response relationship, dose-response curves.

OC(CB4)-30: Principles of Therapeutics

Plasma Drug concentration vs Time profile, Definition and explanation of various terms: MEC, MSC, MTC, AUC(graph). Peak plasma concentration, time of peak concentration. Therapeutic range. Steady state concentration, onset of action, onset of time, duration of action, intensity of action. LD50, ED50. Therapeutic objective. Dosage regimen, Design of dosage regimes: Dose size, dosing frequency, drug accumulation during multiple dosing, time to reach steady-state during multiple dosing, average concentration and body content on multiple dosing to steady state, loading dose, maintenance dose, maintenance of drug within the therapeutic range, design of dosage regimen from plasma concentration. Kinetics of fixed dose, fixed time interval regimes. Modification to dosage regime: Dosing of drugs in obese patients, dosing of drugs in Neonates, infants & children, dosing of drugs in geriatrics (elderly), dosing of drugs in Hepatic disease, dosing of drugs in renal disease.

OC(CB4)-31: Drug Interactions.

Introduction, classification, Mechanisms of drug interactions.– pharmacokinetic interactions(alteration of gastrointestinal absorption, complexation and adsorption, alteration of distribution, alteration of metabolism and alteration of excretion) & pharmacodynamic interactions (antagonistic effects, synergistic effects, alteration of electrolyte levels, interactions involving adrenergic system, alteration of receptor site interaction and antibiotic combinations). Influence of alcohol(Anti biotics, Anti coagulants, Anti histamines, Anti psychotic drugs, sedatives and Hypnotics), smoking(Theophylline, Diazepam, a Tri cyclic antidepressants), food (Bronchodilators, Diuretics, ACE Inhibitors, Anti coagulants, Tetracyclines) on drug action.

Reference books:

1. Pharmacokinetics. By Shobha Rani
2. Elements of Pharmacology. By Gandhi, Desani & Goyal.
3. Goodman & Gilman's "The pharmacological basis of therapeutics. By Gilman & Rali.
4. Pharmacology. By Rang.
5. Biopharmaceutics and pharmacokinetics By Brahmanikar
6. Pharmacology By Lippincott
7. Modern Pharmacology with Clinical Applications. By R. Craig.
8. Comprehensive pharmacy review by Leon Shargel
9. Hospital and clinical pharmacy
10. Burger's medicinal chemistry and drug discovery. By Manfred E. Wolf.
11. Introduction to Medicinal chemistry. By Patrick.
12. Comprehensive medicinal chemistry. Vol 1-5 By Hanzsch.
13. Principles of medicinal chemistry. By William Foye
14. Biochemical approach to medicinal chemistry. By Thomas Nogrady.

Laboratory courses

Paper CH (OC) 451P: Spectroscopic identification of organic compounds & practice of chemistry software programmes

1. Identification of unknown organic compounds by interpretation of IR, UV, ^1H -NMR, ^{13}C NMR, and mass spectral data(two examples with 2D-NMR). A minimum of 30 representative examples should be studied.

2. **Chemistry software programmes:** Chem Draw, analysis of IR and NMR using ACD/Id NMR processor. EXCEL: Drawing graphs, Molecular docking.

Paper CH (OC) 452P: Synthesis and analysis of drugs

(A) Laboratory Synthesis of the following drugs:

Paracetamol, Phenytoin, Benzocaine, 6-Methyluracil, Chloritone, Fluorescein, 4-Aminobenzene sulfonamide, antipyrine and phenothiazine

(B) Estimation of the following drugs:

Aspirin (titrimetry), Ibuprofen (titrimetry), Analgin (titrimetry), Chloride in Ringer's lactate (argentometry), ascorbic acid {titrimetry, Iodometry and Cerimetry}, colorimetry}, Isoniazid(Iodometry), Riboflavin(colorimetry), Zn ions in Bactracin Zinc, Ca^{+2} ions in Calcium gluconate injection(complexometry), Riboflavin (UV-Visible Spectrophotometer).

Reference books:

1. Practical organic chemistry by Mann & Saunders
2. Text book of practical organic chemistry by Vogel
3. The systematic identification of organic compounds by Shriner et.al
4. Analytical chemistry by G N David Krupadanam et.al
5. Advanced practical medicinal chemistry by Ashutoshkar
6. Pharmaceutical drug analysis by Ashutoshkar
7. Quantitative analysis of drugs in pharmaceutical formulations by P D Sethi
8. Practical pharmaceutical chemistry part-1 and part-2 by A H Beckett and J B Stenlake
9. Spectroscopic identification of organic compounds by R M Silverstein and F X Webster