Department of Pharmaceutical Chemistry, Telangana University 5yrs Integrated M.Sc Chemistry (Pharmaceutical Chemistry) Syllabus for I and II Semesters

The following syllabus for **5yrs Integrated M.Sc Chemistry (Pharmaceutical Chemistry)** was unanimously approved by board of studies in its meeting held at Department of Pharmaceutical Chemistry, Telangana University, Nizamabad on 13th July, 2015.

Yr	Sem	Sem Paper Code	Subject	hrs/	M	arks	Duration of exam in hrs		Credits
		Code	, and the second	week	IE*	UE**	IE*	UE**	
I	I	IPCH-1.1T	English-I	4	30	70	1	3	4
		IPCH-1.2T	Second language (Telugu/ Hindi)-I	4	30	70	1 /	3	4
		ІРСН-1.3Т	Atomic structure, bonding, general organic chemistry & aliphatic hydrocarbons	4	30	70	Î	3	4
		IPCH-1.4T	Basics of pharmaceutical sciences	4	30	70 (9 1	3	4
		IPCH-1.5T	Microbiology and immunology	4	30	70	1	3	4
		IPCH-1.3Lab	Inorganic and organic chemistry lab	3	15	35	3	3	2
		IPCH-1.4Lab	Pharmaceutical sciences lab	3	15	35	3	3	2
		IPCH-1.5Lab	Microbiology and immunology lab	3	15	35	3	3	2
				21***	195	455			26
I	II	IPCH-2.1T	English-II	4	30	70	1	3	4
		IPCH-2.2T	Second language (Telugu/ Hindi)-II	4	30	70	1	3	4
		ІРСН-2.3Т	Chemical energetics, states of matter & functional group organic chemistry	4	30	70	1	3	4
		IPCH-2.4T	Anatomy and physiology	4	30	70	1	3	4
		IPCH-2.5T	Biochemistry	4	30	70	1	3	4
		IPCH-2.3Lab	Physical and organic chemistry lab	3	15	35	3	3	2
		IPCH-2.4Lab	Anatomy and physiology lab	3	15	35	3	3	2
		IPCH-2.5Lab	Biochemistry lab	3	15	35	3	3	2
			2.0	21***	195	455			26
			Total Marks (I and I	II Sem)	1.	300	Total	Credits	52

^{***}English and SL (each 4 hrs/week) work load not included here; **University Examination; *Internal Examination

S.No	Name	Designation
1	Dr. V. Chandrasekhar, Dept. of Pharmaceutical Chemistry, Telangana University	Chairman
2	Dr. B. Shireesha, Dept. of Pharmaceutical Chemistry, Telangana University	Ex-officio Member
3	Prof. Naseem, Dept. of Pharmaceutical Chemistry, Telangana University	Member
4	Dr. M. Satyanarayana, Dept. of Pharmaceutical Chemistry, Telangana University	Member
5	Prof. Ch. Krishna Reddy, Dept. of Chemistry, Osmania University	Member
6	Prof. V. Ravinder, Dept. of Chemistry, Kakatiya University	Member
7	Prof. C. Veeresham, UCPSc, Kakatiya University	Member
8	Dr. B. Prabhasankar, Leads Pharma Pvt. Ltd, Hyderabad	Member
9	Prof. A. K. D. Bhavani, Dept. of Chemistry, Osmania University	Member
10	Prof. Devadas, Dept. of Chemistry, Osmania University	Member
11	Prof. Veerasomaiah, Dept. of Chemistry, Osmania University	Member
12	Dr. P. Jalapathi, Dept. of Chemistry, Osmania University	Member
13	Dr. A. Hari Padma Sree, Dept. of Chemistry, Koti Women's Coll., OU	Member

Department of Pharmaceutical Chemistry, Telangana University 5yrs Integrated M.Sc Chemistry (Pharmaceutical Chemistry) Syllabus for III and IV Semesters

The following syllabus for **5yrs Integrated M.Sc Chemistry (Pharmaceutical Chemistry)** was unanimously approved by board of studies in its meeting held at Department of Chemistry, Osmania University, Hyderabad on 27th June, 2016.

Yr		Sam Paper	Subject	hrs/		arks	Dura	ation of n in hrs	Credits
	bem	Code	Subject	week	IE*	UE**	IE*	UE**	Crearis
II	III	IPCH-3.1T	English-III	4	30	70	1	3	4
		IPCH-3.2T	Environmental science	4	30	70	1	3	4
		ІРСН-3.3Т	Solutions, electrochemistry & functional group organic chemistry	4	30	70	1	3	4
		IPCH-3.4T	Pharmaceutical analysis	4	30	70	1	3	4
		IPCH-3.5T	Cell and molecular biology	4	30	70	1	3	4
		IPCH-3.3Lab	Physical chemistry and organic chemistry lab	3	15	35	3	3	2
		IPCH-3.4Lab	Pharmaceutical analysis lab	3	15	35	3	3	2
		IPCH-3.5Lab	Cell and molecular biology lab	3	15	35	3	3	2
				25***	195	455			26
II	IV	IPCH-4.1T	English-IV	4	30	70	1	3	4
		ІРСН-4.2Т	Chemistry of nutraceuticals and dairy products	4	30	70	1	3	4
		ІРСН-4.3Т	Coordination chemistry, chemical kinetics, dilute solutions & colligative properties, colloids & surface chemistry	4	30	70	1	3	4
		IPCH-4.4T	Pharmacology-I	4	30	70	1	3	4
		IPCH-4.5T	Genetic engineering and its applications in pharmaceutical sciences	4	30	70	1	3	4
		IPCH-4.3Lab	Inorganic and physical chemistry lab	3	15	35	3	3	2
		IPCH-4.4Lab	Pharmacology lab	3	15	35	3	3	2
		IPCH-4.5Lab	Genetic engineering lab	3	15	35	3	3	2
				25***	195	455			26
			Total Marks (III and I	V Sem)	1	300	Total	Credits	52

^{***}English work load (4 hrs/week) not included here; **University Examination; *Internal Examination

S.No	Name	Designation
1	Dr. V. Chandrasekhar, Dept. of Pharmaceutical Chemistry, Telangana University	Chairman
2	Dr. B. Shireesha, Dept. of Pharmaceutical Chemistry, Telangana University	Ex-officio Member
3	Prof. Naseem, Dept. of Pharmaceutical Chemistry, Telangana University	Member
4	Dr. M. Satyanarayana, Dept. of Pharmaceutical Chemistry, Telangana University	Member
5	Prof. Ch. Krishna Reddy, Dept. of Chemistry, Osmania University	Member
6	Prof. V. Ravinder, Dept. of Chemistry, Kakatiya University	Member
7	Prof. C. Veeresham, UCPSc, Kakatiya University	Member
8	Dr. S. Ramakrishna, IICT, Hyderabad	Member
9	Prof. Devadas, Dept. of Chemistry, Osmania University	Member
10	Prof. Veerasomaiah, Dept. of Chemistry, Osmania University	Member
11	Dr. P. Jalapathi, Dept. of Chemistry, Osmania University	Member
12	Dr. A. Hari Padma Sree, Dept. of Chemistry, Koti Women's Coll., OU	Member

Department of Pharmaceutical Chemistry, Telangana University 5yrs Integrated M.Sc Chemistry (Pharmaceutical Chemistry) Syllabus for V and VI Semesters

The following syllabus for **5yrs Integrated M.Sc Chemistry (Pharmaceutical Chemistry)** was unanimously approved by board of studies in its meeting held at Department of Chemistry, Osmania University, Hyderabad on 19th Sept, 2017

Yr	Sem	Paper Code	Subject	hrs/ week		arks UE**	Dura	tion of in hrs UE**	Credits
III	V	IPCH-5.1T	Physical chemistry and topics of industrial importance	4	30	70	1	3	4
		IPCH-5.2T	Coordination and supramolecular chemistry	4	30	70	1	37)	4
		IPCH-5.3T	Principles of drug discovery and development	4	30	70	1	3	4
		IPCH-5.4T	Molecular targets and signal transduction	4	30	70	⁹ 1	3	4
		IPCH-5.5T	Principles of stereochemistry	4	30	70	1	3	4
		IPCH-5.3Lab	Principles of drug discovery and development lab	3	15	35	3	3	2
		IPCH-5.4Lab	Molecular targets and signal transduction lab	3	15	35	3	3	2
		IPCH-5.5Lab	Organic synthesis lab	3	15	35	3	3	2
				29	195	455			26
III	VI	IPCH-6.1T	Reagents and reaction mechanism	4	30	70	1	3	4
		IPCH-6.2T	Inorganic chemistry	4	30	70	1	3	4
		ІРСН-6.3Т	Quality control of bulk drugs and formulations	4	30	70	1	3	4
		IPCH-6.4T	Spectroscopic techniques	4	30	70	1	3	4
		IPCH-6.5T	Quantum chemistry, electrochemistry and polymers	4	30	70	1	3	4
		IPCH-6.3Lab	Pharmaceutical chemistry lab	3	15	35	3	3	2
		IPCH-6.4Lab	Spectroscopy lab	3	15	35	3	3	2
		IPCH-6.5Lab	Physical chemistry lab	3	15 195	35	3	3	2
						455			26
Total Marks (V and VI Sem) 1300 To								Credits	52

University Examination; *Internal Examination

	is present in the bourt of studies meeting herd.						
S.No	Name	Designation					
1	Prof. Naseem, Dept. of Pharmaceutical Chemistry, Telangana University	Chairman					
2	Dr. V. Chandrasekhar, Dept. of Pharmaceutical Chemistry, Telangana University	Ex-Officio Member					
3	Dr. B. Shireesha, Dept. of Pharmaceutical Chemistry, Telangana University	Member					
4	Dr. M. Satyanarayana, Dept. of Pharmaceutical Chemistry, Telangana University	Member					
5	Prof. C. Veeresham, UCPSc, Kakatiya University	Member					
6	Prof. V. Ravinder, Dept. of Chemistry, Kakatiya University	Member					

Department of Pharmaceutical Chemistry, Telangana University 5yrs Integrated M.Sc Chemistry (Pharmaceutical Chemistry) Syllabus for VII and VIII Semesters

The following syllabus for **5yrs Integrated M.Sc Chemistry (Pharmaceutical Chemistry)** was unanimously approved by board of studies in its meeting held at Department of Pharmaceutical Chemistry, Telangana University, Nizamabad on 9th May, 2018.

Yr	Sem	Paper Code	Subject	hrs/ week	Ma	arks		tion of in hrs	Credits
		Code		week	IE*	UE**	IE*	UE**	
IV	VII	IPCH-7.1T	Spectroscopy-II	4	30	70	1	3	4
		IPCH-7.2T	Advanced organic synthesis-I	4	30	70	1	3	4
		IPCH-7.3T	Medicinal chemistry-I	4	30	70	1	3	4
		IPCH-7.4T	Bioinorganic and physical chemistry	4	30	70	1	3	4
		IPCH-7.2Lab	Organic chemistry lab	6	15	35	3	3	2
		IPCH-7.3Lab	Medicinal chemistry lab	6	15	35	7 3	3	2
		IPCH-7.4Lab	Inorganic and physical lab	6	15	35	3	3	2
				34	165	385			22
IV	VIII	IPCH-8.1T	Pharmaceutical chemistry	4	30	70	1	3	4
		IPCH-8.2T	Heterocyclic chemistry	4	30	70	1	3	4
		IPCH-8.3T	Medicinal chemistry-II	4	30	70	1	3	4
		IPCH-8.4T	Physical and general chemistry	4	× 30	70	1	3	4
		IPCH-8.1Lab	Organic chemistry lab	6	15	35	3	3	2
		IPCH-8.2Lab	Spectroscopy lab	6	15	35	3	3	2
		IPCH-8.3Lab	Pharmaceutical chemistry lab-I	6	15	35	3	3	2
		IPCH-8.4MP	Mini project	4	-	100	-	-	4
				38	165	485			26
		<u> </u>	Total Marks (VII and VI	II Sem)	12	200	Total	Credits	48

^{**}University Examination; *Internal Examination

Mini project: Each student has to submit a project report on literature review/minor research project at the end of the semester

S.No	Name	Designation
1	Prof Naseem, Dept. of Pharmaceutical Chemistry, Telangana University	Chairman
2	Dr V Chandra Sekhar, Dept. of Pharmaceutical Chemistry, Telangana University	Ex-officio Member
3	Dr. B. Shireesha, Dept. of Pharmaceutical Chemistry, Telangana University	Member
4	Dr. M. Satyanarayana, Dept. of Pharmaceutical Chemistry, Telangana University	Member
5	Prof. V. Ravinder, Dept. of Chemistry, Kakatiya University	Member
6	Prof. C. Veeresham, UCPSc, Kakatiya University	Member
7	Prof. Veerasomaiah, Dept. of Chemistry, Osmania University	Member

Department of Pharmaceutical Chemistry, Telangana University 5yrs Integrated M.Sc Chemistry (Pharmaceutical Chemistry) Syllabus for IX and X Semesters

The following syllabus for **5yrs Integrated M.Sc Chemistry (Pharmaceutical Chemistry)** was unanimously approved by board of studies in its meeting held at Department of Pharmaceutical Chemistry, Telangana University, Nizamabad on 30th July, 2019

Yr	Sem	Paper Code	Simieri	hrs/ week	M	arks	Duration of exam in hrs		Credits
		Code		WEEK	IE*	UE**	IE*	UE**	
V	IX	IPCH-9.1T	Pericyclic and photochemistry	4	30	70	1	3	4
		ІРСН-9.2Т	Organometallics, homogeneous catalysis and advanced organic synthesis-II	4	30	70	1	3	4
		IPCH-9.3T	Natural products	4	30	70	1	3	4
		IPCH-9.4T	Modern drug synthesis	4	30	70	1	3	4
		IPCH-9.5T	Molecular modelling and drug design	4	30	70	1	3	4
		IPCH-9.3Lab	Natural products lab	6	15.	35	3	3	2
		IPCH-9.4Lab	Peptide chemistry lab	6	15	35	3	3	2
		IPCH-9.5Lab	Molecular modeling & drug design lab	6	15	35	3	3	2
				38	195	455			26
V	X	IPCH-10	Major project	36	#50	##400	Viva	-Voce	18
	Total Marks (IX and X Sem) 1100 Total Credits								

^{**}University Examination; *Internal Examination

S.No	Name	Designation
1	Dr. B. Shireesha, Dept. of Pharmaceutical Chemistry, Telangana University	Chairman
2	Dr. M. Satyanarayana, Dept. of Pharmaceutical Chemistry, Telangana University	Ex-officio Member
3	Prof Naseem, Dept. of Pharmaceutical Chemistry, Telangana University	Member
4	Dr V. Chandra Sekhar, Dept. of Pharmaceutical Chemistry, Telangana University	Member
5	Prof. G. Achaiah, UCPSc, Kakatiya University	Member
6	Dr. M. Vasantha, Dept. of Chemistry & Pharmaceutical Sci., Mahatma Gandhi University	Member
7	Ms. M. Prasanna Sheela, Dept. of Biotechnology, Telangana University	Member

Year	Semester	Hours/Week	Ma	rks	Credits	
rear	Semester		IE	UE	Creans	
I	I	[#] 29	195	455	26	
I	II	[#] 29	195	455	26	
II	III	^{\$} 29	195	455	26	
II	IV	^{\$} 29	195	455	26	
III	V	29	195	455	26	
III	VI	29	195	455	26	
IV	VII	34	165	385	22	
IV	VIII	38	165	485	26	
V	IX	38	195	455	26	
V	X	36	50	400	18	
		Total	62	00	248	

[#]Including Telugu and English work load (4+4); *Including English work load (4)

^{*50} Marks for design seminar; ##200 marks for presentation & 200 marks for defence and comprehensive viva

SEMESTER-I

IPCH-1.3T: ATOMIC STRUCTURE, BONDING, GENERAL ORGANIC CHEMISTRY & ALIPHATIC HYDROCARBONS

(Units: 5, Hours: 60, Credits: 4)

Unit-I: Atomic Structure

Review of Bohr's theory and its limitations, dual behavior of matter and radiation, de-Broglie's relation, Heisenberg Uncertainty principle. Hydrogen atom spectra, Need of a new approach to Atomic structure.

What is Quantum mechanics? Time independent Schrodinger equation and meaning of various terms in it, Significance of ψ and ψ^2 , Schrödinger equation for hydrogen atom, Radial and angular parts of the hydrogenic wave functions (atomic orbitals) and their variations for 1s, 2s, 2p, 3s, 3p and 3d orbitals (Only graphical representation), Radial and angular nodes and their significance, Radial distribution functions and the concept of the most probable distance with special reference to 1s and 2s atomic orbitals, Significance of quantum numbers, orbital angular momentum and quantum numbers m_1 and m_s , Shapes of s, p and d atomic orbitals, nodal planes, Discovery of spin, spin quantum number (s) and magnetic spin quantum number (m_s)

Rules for filling electrons in various orbitals, Electronic configurations of the atoms, Stability of half-filled and completely filled orbitals, concept of exchange energy, Relative energies of atomic orbitals, Anomalous electronic configuration.

Unit-II: Chemical Bonding and Molecular Structure-I

Ionic Bonding: General characteristics of ionic bonding. Energy considerations in ionic bonding, lattice energy and solvation energy and their importance in the context of stability and solubility of ionic compounds, Statement of Born-Landé equation for calculation of lattice energy, Born -Haber cycle and its applications, polarizing power and polarizability. Fajan's rules, ionic character in covalent compounds, bond moment, dipole moment and percentage ionic character.

Unit-III: Chemical Bonding and Molecular Structure-II

Covalent bonding: Valence bond theory, Shapes of some inorganic molecules and ions on the basis of VSEPR and hybridization with suitable examples of linear, trigonal planar, square planar, tetrahedral, trigonal bipyramidal and octahedral arrangements

Concept of resonance and resonating structures in various inorganic and organic compounds

MO Approach: Rules for the LCAO method, bonding and antibonding MOs and their characteristics for s-s, s-p and p-p combinations of atomic orbitals, nonbonding combination of orbitals, MO treatment of homonuclear diatomic molecules of 1st and 2nd periods (including idea of s-p mixing) and heteronuclear diatomic molecules such as CO, NO and NO⁺. Comparison of VB and MO approaches.

Unit-IV: Fundamentals of Organic Chemistry

Brief review of structural theory of organic chemistry, hybridization, bond length, bond angle, bond energy; inductive effect, electromeric effect, resonance, hyperconjugation, and their application in the analysis of strength of organic acids, bases and stability of organic compounds; structure, shape and reactivity of nucleophiles, electrophiles and free radicals; cleavage of bonds-homolysis and heterolysis **Types of organic reactions:** Addition reactions-electrophilic, nucleophilic and free radical; Substitution reactions-electrophilic, nucleophilic and free radical; elimination and rearrangement reactions

Unit-V: Aliphatic Hydrocarbons

Functional group approach for the following reactions (preparations & reactions) to be studied in context to their structure

Alkanes: Preparation: Catalytic hydrogenation, Wurtz reaction, Kolbe's synthesis, from Grignard reagent. Reactions: Free radical Substitution: Halogenation, Synthesis of cycloalkanes and different kinds of strains in cycloalkanes

Alkenes: Preparation: Elimination reactions: Dehydration of alkenes and dehydrohalogenation of alkyl halides (Saytzeff's rule); cis alkenes (Partial catalytic hydrogenation) and trans alkenes (Birch reduction). Reactions: cis-addition (alk. KMnO4) and trans-addition (bromine), Addition of HX (Markownikoff's and anti-Markownikoff's addition), Hydration, Ozonolysis, oxymecuration-demercuration, Hydroboration-oxidation

Alkynes: Preparation: Acetylene from CaC₂ and conversion into higher alkynes; by dehalogenation of tetra halides and dehydrohalogenation of vicinal-dihalides. Reactions: formation of metal acetylides, addition of bromine and alkaline KMnO₄, ozonolysis and oxidation with hot alk, KMnO₄

- 1. J. D. Lee: A new Concise Inorganic Chemistry, E L. B. S.
- 2. F. A. Cotton & G. Wilkinson: Basic Inorganic Chemistry, John Wiley.
- 3. Douglas, McDaniel and Alexader: Concepts and Models in Inorganic Chemistry, John Wiley.
- 4. James E. Huheey, Ellen Keiter and Richard Keiter: Inorganic Chemistry: Principles of Structure and Reactivity, Pearson Publication.
- 5. T. W. Graham Solomon: Organic Chemistry, John Wiley and Sons.
- 6. Peter Sykes: A Guide Book to Mechanism in Organic Chemistry, Orient Longman.
- 7. E. L. Eliel: Stereochemistry of Carbon Compounds, Tata McGraw Hill.
- 8. I. L. Finar: Organic Chemistry (Vol. I & II), E. L. B. S.
- 9. R. T. Morrison & R. N. Boyd: Organic Chemistry, Prentice Hall.
- 10. Arun Bahl and B. S. Bahl: Advanced Organic Chemistry, S. Chand.

IPCH-1.4T: BASICS OF PHARMACEUTICAL SCIENCES

(Units: 5, Hours: 60, Credits: 4)

Basic introduction to the following topics in each unit

Unit-I: Scope of Pharmaceutical Sciences

Origin, development and scope of chemical sciences, pharmaceutical sciences, introduction to the fundamentals of pharmaceutical sciences, basic introduction, definitions, significance and interdisciplinary relevance of following in pharmaceutical sciences: Inorganic chemistry, organic chemistry, physical chemistry, analytical chemistry, biochemistry, statistics, microbiology, immunology, anatomy and physiology, pharmacology, pharmacognosy, phytochemistry, medicinal chemistry, pharmaceutical chemistry, pharmaceutics, biopharmaceutics pharmacokinetics, clinical pharmacy/ pharmacy practice, food technology, cosmetic technology, toxicology, informatics.

Unit-II: Drugs and Pharmaceuticals

History and evolution of drugs, Ayurveda, Homeopathy, Unani, Siddha and Allopathy systems of medicine, advantages and limitations of various systems of medicine, Definition and nomenclature of pharmaceuticals, generic and trade names, source and classification of drugs based on therapeutic action, General mechanism and factors affecting drug action, pharmacodynamics, pharmacokinetics (ADME), bioavailability, agonism, antagonism, synergism, adverse reactions, Drug dependences, drug abuse, drug tolerance, hypersensitivity/ anaphylaxis.

Unit-III: Drug Discovery

Introduction to stages of drug discovery and development, lead, pharmacophore, serendipity, specific, nonspecific drugs, drug targets, activity and affinity of drugs, measurement and units of drug activity, potency of drugs, effect of concentration on activity, factors effecting drug dosage, physico-chemical factors affecting drug action, natural, semisynthetic and synthetic drugs with examples.

Unit-IV: Drug Formulations

Introduction to dosage forms, their classification with examples, routes of administration, advantages and limitations of specific dosage forms, Ayurveda, Homeopathy, Unani and Siddha formulations, Introduction, classification and uses of following additives in formulation of different dosage forms: preservatives, antioxidants, surfactants, hydrocolloids, emulsifying agents, suspending agents, diluents, binders, lubricants, and organoleptic additives.

Unit-V: Quality Control of Pharmaceuticals

Introduction to Pharmacopoeias-IP, BP, USP & International Pharmacopoeia, National Formularies and Extra Pharmacopoeia; Typical parts of a monograph of Indian pharmacopoeia with examples, quality control and quality assurance, introduction to GLP, GMP, Laboratory Accreditation, quality estimation of aspirin, acetaminophen, isoniazid, ascorbic acid, codeine phosphate, Chloride in Ringers lactate, ethambutol.

- 1. Allen, Loyd V., Jr and Howard C. Ansel: Ansel's Pharmaceutical Dosage Forms and Drug Delivery Systems, 9th Edition, Wolters Kluwer Health publisher.
- 2. Gareth Thomas: Med Chem: An Introduction (Kindle Edition), Wiley India Pvt Ltd; 2nd Edn.
- 3. Brahmankar, D.M and Sunil B. Jaiswal: Biopharmaceutics and Pharmacokinteics.

Syllabus for 5yrs Integrated M.Sc Chemistry (Pharmaceutical Chemistry), Effective from AY 2015-16 Department of Pharmaceutical Chemistry, Telangana University, Dichpally, Nizamabad-503322

- 4. Mehta, R. M: Dispensing and General Pharmacy.
- 5. Tripathi, K. D: Essentials of Medicinal Pharmacology; 6th Edition.
- 6. Indian Pharmacopoeia.
- 7. Kokate: Pharmacognosy.
- 8. John H Block; John M Beale: Wilson and Gisvold's textbook of organic medicinal and epartinent of Pharmaceutical Chemistry, perartinent of Pharmaceutical Chemistry, perartinent of Pharmaceutical Chemistry, and the perar pharmaceutical chemistry, 11th edn.

IPCH-1.5T: MICROBIOLOGY AND IMMUNOLOGY

(Units: 5, Hours: 60, Credits: 4)

Unit-I: Microbial World and Microscopy

History, Scope, Future prospective of Microbiology and its application in Pharmaceutical sciences, Cell as a basic unit of life- Ultra structure of Prokaryotic cell, Ultra structure of Eukaryotic cell, Outline of classification of microorganisms, Characteristic features and economical importance of Algae, Fungi, Actinomycetes; Viruses – Structure, Classification, Medical importance; Principles of Microscopy - Light microscopy, Preparation and staining of specimens: Fixation, Dyes, Staining methods- Simple staining, Differential staining: Gram's staining, Acid-fast staining, Staining specific structures: Endospore, Capsule and Flagella staining, Fluorescent microscope, Phase contrast microscope, Confocal microscope and Electron microscope.

Unit-II: Microbial Nutrition, Culture and Growth

Culture Media, Classification and different types of media, Culture of microorganisms-Pure culture techniques and Aseptic techniques, Maintenance and preservation of Microorganisms, Microbial growth requirements, Nutritional groups of microorganisms, Bacterial growth: Bacterial cell division-Binary fission, Growth of bacterial populations: Growth curve and Growth kinetics, Measurement of growth: Direct and Indirect methods, Influence of environmental factors on Microbial growth-Temperature, pH, Osmolality and Oxygen, Cultivation of Viruses, Life cycle of Viruses: Lytic and Lysogeny

Unit-III: Microbial Growth Control

Concepts of sterilization, Physical methods of sterilization-Heat, Radiation, Filtration, Chemical agents of sterilization-Phenols and Phenolics, Alcohols, Halogens, Aldehydes, Organic acids, Surface active agents, Oxidizing agents, Gaseous agents, Evaluation of the efficiency of sterilization methods, sterility indicators, factors affecting the microbial spoilage, sources, types of microbial contaminants of pharmaceutical products, evaluation of microbial stability of formulations, Sterility testing of parenteral formulations - solids, liquids, ophthalmic and other sterile products according to the I.P., sterility testing of sterile surgical devices, Disinfectants, Sanitizers, Antiseptics and antimicrobial agents (antibacterial agents, antiviral agents, antibiotics) Effect of antimicrobial agents on Microbial growth, Measurement of antimicrobial activity (MIC), Preservation of pharmaceutical products using antimicrobial agents.

Unit-IV: Immunology

History and Concepts of immunity, Cells and Organs of the immune system, Properties of Antigens-Epitope, Hapten, Adjuvants, Structure and different classes of immunoglobulins, Cell and humoral mediated immunity, Hypersensitivity, types of allergic reactions, Antigen - Antibody reactions: Agglutination, Precipitation, Neutralization, Complement fixation, ELISA, Radioimmuno assay, Immunoblotting; Autoimmune disorders – Hashimoto's Thyroiditis, Autoimmune anemia, Insulin dependent Diabetes Mellitus, Systemic lupus erythematosus, Rheumatoid arthritis.

Unit-V: Epidemiology

Terminology of Epidemics-Sporadic, endemic, hyperendemic, outbreak, epidemic and pandemic; Tools of epidemics-Morbidity rate, prevalence rate, mortality; Recognition of an infectious disease in a population, Recognition of an epidemic; the infectious disease cycle-pathogen and reservoir; Modes of transmission of pathogen; Airborne bacterial diseases- Tuberculosis, Diphtheria, viral diseases-

Chicken pox and Shingles, Flu; Water and foodborne bacterial diseases- Typhoid, Cholera, viral diseases-Polio, Hepatitis; Diseases caused by direct contact: bacterial-Leprosy, Gas gangrene, viral-AIDS, Coldsores: Zoonotic diseases: bacterial-Anthrax, Brucellosis, viral- Rabies, Ebola; Arthopod borne diseases: bacterial-Plague, Typhus fever, viral-Encephalitis, Yellow fever; Control of epidemics Vaccines and immunization

- 1. Thomas D. Brock: Biology of Microorganisms.
- 2. Prescott's Microbiology.
- 3. Gerard J. Tortora and Berdell R. Funke: Microbiology, An introduction.
- 4. Michael J. Pelczar: Microbiology.
- 5. Ananthanarayan and Paniker's Textbook of Microbiology.
- 6. Dr. C. B. Powar and Dr. H. F. Daginawala: General Microbiology.
- 7. Thomas J. Kindt, Barbara A. Osborne, Richard A. Goldsby: Kuby Immunology.
- 8. Peter J. Delves, Seamus J. Martin, Dennis R. Burton, Ivan M. Roitt: Essential Immunology.
- 9. Fahim Halim Khan: Elements of Immunology.
- 10. Rastogi S. C: Elements of Immonology.

IPCH-1.3LAB: INORGANIC AND ORGANIC CHEMISTRY LAB (Credits: 2, 3hrs/week)

Section-A: Inorganic Chemistry-Volumetric Analysis

- 1. Estimation of sodium carbonate and sodium hydrogen carbonate present in a mixture.
- 2. Estimation of oxalic acid by titrating it with KMnO₄.
- 3. Estimation of water of crystallization in Mohr's salt by titrating with KMnO₄.
- 4. Estimation of Fe (II) ions by titrating it with $K_2Cr_2O_7$ using internal indicator.
- 5. Estimation of Cu (II) ions iodometrically using Na₂S₂O₃.

Section-B: Organic Chemistry

- 1. Solubility test of organic compounds in different test solvents & solutions
- 2. Detection of extra elements (N, S, Cl, Br, I) in organic compounds (containing up to two extra elements)
- 3. Separation of mixtures by Thin Layer Chromatography: Measure the R_f value in each case Identify and separate the components of a given mixture of 2 amino acids (glycine, aspartic acid, glutamic acid, tyrosine or any other amino acid) by paper chromatography

- 1. Vogel's Qualitative Inorganic Analysis, A.I. Vogel, Prentice Hall, 7th Edition.
- 2. Vogel's Quantitative Chemical Analysis, A.I. Vogel, Prentice Hall, 6th Edition.
- 3. Textbook of Practical Organic Chemistry, A.I. Vogel, Prentice Hall, 5th edition
- 4. Practical Organic Chemistry, F. G. Mann. & B. C. Saunders, Orient Longman, 1960

IPCH-1.4LAB: PHARMACEUTICAL SCIENCES LAB (Credits: 2, 3hrs/week)

A brief introduction to laboratory safety, types and quality of glassware, chemicals, errors, classification of errors, accuracy and precision, minimization of errors, weighing methods, sensitivity, calibration and standard operating procedures (SOP's) of instruments (glassware, balance) with examples, normality, molality, molarity, percentage calculations, % W/V, V/V & W/W, ppm, ppb, inter conversions, isotonicity and pH of solutions with examples,

- 1. Preparation and dilution of solutions
- 2. Weighing of solid, liquid substances
- 3. Weight variation analysis of tablets
- 4. Preparation and labelling of moisturizing lotion
- 5. Effect of suspending agent on stability of suspensions
- 6. Calibration of instruments: burette, pipette, balance, thermometer, volumetric flask.
- 7. Preparation of neutral, acidic and basic phosphate buffers
- 8. Generation of drug libraries using softwares
- 9. Identification of pharmacophoric features and lead molecules from various drugs
- 10. Effect of solubility and concentration on activity of compounds
- 11. Estimation and comparison of potency of any two inorganic antacids available in market
- 12. Determination of IC₅₀ from activity data of compounds
- 13. Extraction of caffeine from tea leaves
- 14. Preparation and application of Triphala churna powder
- 15. Preparation of herbal tea for reduction of fat content
- 16. Monograph analysis of paracetamol tablets

- 1. Allen, Loyd V., Jr, Remington: the Science and Practice of Pharmacy, 22nd Edn, Pharmaceutical Press.
- 2. Sidney James Carter, Cooper and Gunn's Tutorial Pharmacy, 6th Edn, Pitman Medical Publishers.
- 3. J. Mendham and R. C. Denney: Vogel's Quantitation Chemical Analysis, 6th Edn, Prentice Hall
- 4. A. H. Beckett and J. B. Stenlake: Practical Pharmaceutical Analysis, Part 1, 4th Edn, Continuum International-Athlone Publishers..

IPCH-1.5LAB: MICROBIOLOGY AND IMMUNOLOGY LAB (Credits: 2, 3hrs/week)

- 1. Concepts of microscopy
- 2. Sterilization techniques
- 3. Microbiological media preparation-Nutrient Agar, Nutrient Broth
- 4. Isolation of pure cultures Spread plate method, Streak plate method, Pour plate method
- 5. Simple staining of Bacteria
- 6. Gram's staining of Bacteria
- 7. Turbidometric estimation of bacterial growth
- 8. Effect of temperature on bacterial growth
- 9. Effect of pH on bacterial growth
- 10. Isolation of Fungi
- 11. Microscopic observation of Fungi by fungal mounting
- 12. Isolation of Algae
- 13. Rideal-Walker test
- 14. Widal test
- 15. Microscopic observation of permanent slides of Algae and Fungi
- 16. Study of symptoms of viral diseases

- 1. Gopal Reddy et al: Laboratory Experiments in Microbiology.
- 2. Arthi Nigam and Archana Ayyagari: Lab manual in Biochemistry, Immunology and Biotechnology.

SEMESTER-II

IPCH-2.3T: CHEMICAL ENERGETICS, STATES OF MATTER AND FUNCTIONAL GROUP ORGANIC CHEMISTRY

(Units: 5, Hours: 60, Credits: 4)

Unit-I: Thermodynamics-I

Thermodynamic system and surroundings, thermodynamic processes; Extensive and Intensive properties, State and path function, Internal energy, Work and Heat; Internal energy a state function and exact differential; Work and Heat path functions and inexact differentials

First Law of thermodynamics-Statement and Mathematical expression-its various forms

Reversible and Irreversible process; Pressure-Volume work; Derivation of expression for maximum work done in reversible isothermal expansion of an Ideal gas, work done in irreversible isothermal expansion of Ideal gas-Problems. Derivation of expression for work done in reversible adiabatic expansion of an Ideal gas-Comparison between reversible isothermal and adiabatic expansion of an ideal gas, PV⁷=Constant for adiabatic changes. P,V curves for isothermal and adiabatic process

Enthalpy-Heat of reaction at constant volume and constant pressure, Heat capacity-Heat capacities at constant volume and constant pressure, Derive Cp-Cv=R

Variation of Heat of reaction with temperature-Kirchoff's equation and problems

Limitations of First law of thermodynamics and need for Second law; Statement of Second law of thermodynamics-its various statements; Conversion of heat into work- Carnot cycle and efficiency of heat engine-Carnot Theorem-problems

Concept of Entropy-entropy as a state function-Entropy changes in i) reversible process iii) Irreversible process iii) phase changes iv) Reversible isothermal expansion

Free energy Gibbs function and Helmholtz function; Criteria for spontaneity in terms of Gibbs free energy change; Derivation of Gibbs-Helmholtz equation and its significance

Unit-II: Gaseous and Solid State Chemistry

Gaseous State: Deviation of real gases from ideal behavior; van der Waals equation of state; Critical phenomenon; PV isotherms of real gases, continuity of state; Andrew's isotherms of CO₂; The van der Waal's equation and critical state; Derivation of relationship between critical constants and van der Waal's constants; The law of corresponding states, reduced equation of states; Joule Thomson effect and inversion temperature of a gas; Liquifaction of gases: i) Linde's method based on Joule Thomson effect ii) Claude's method based on adiabatic expansion of a gas

Solid State: Laws of Crystallography-(i) Law of Constancy of interfacial angles (ii) Law of Symmetry, Symmetry elements in crystals (iii) Law of rationality of indices; Definition of space lattice, unit cell; Bravis Lattices and seven crystal systems (a brief review); X-ray diffraction by crystals; Derivation of Bragg's equation and its application in the determination of structure of NaCl, KCl & CsCl (Bragg's method and Powder method); Frenkel and Shottky defects. Band structure of solids

Unit-III: Benzene, Alkyl and Aryl Halides

Benzene: Preparations: from phenol, by decarboxylation, from acetylene, from benzene sulphonic acid. Reactions (Case benzene): Orientation in aromatic substitution reactions (ring activation and ring deactivation) Electrophilic substitution (with mechanism) reactions nitration, halogenation and sulphonation, Friedel-Craft's reaction (alkylation and acylation), Side chain oxidation of alkyl benzenes, Aromaticity: Benzenoids and Hückel's rule

Alkyl Halides: Types of Nucleophilic Substitution $(S_N1, S_N2 \text{ and } S_Ni)$ reactions; Preparation: from alkenes and alcohols. Reactions: hydrolysis, nitrite & nitro formation, nitrile & isonitrile formation.

Williamson's ether synthesis: Elimination Vs substitution.

Aryl Halides: Preparation: (Chloro, bromo and iodo-benzene case): from phenol, Sandmeyer & Gattermann reactions. Reactions (Chlorobenzene): Aromatic nucleophilic substitution (replacement by -OH group) and effect of nitro substituent. Benzyne Mechanism: KNH₂/NH₃ (or NaNH₂/NH₃). Reactivity and Relative strength of C-Halogen bond in alkyl, allyl, benzyl, vinyl and aryl halides.

Unit-IV: Alcohols, Phenols and Ethers

Alcohols: Preparation: Preparation of 1°, 2° and 3° alcohols: using Grignard reagent, Ester hydrolysis, Reduction of aldehydes, ketones, carboxylic acid and esters. Reactions: With sodium, HX (Lucas test), esterification, oxidation (with PCC, alk. KMnO₄, acidic dichromate, conc. HNO₃), Oppeneauer oxidation Diols: (Upto 6 Carbons) oxidation of diols. Pinacol-Pinacolone rearrangement

Phenols: Preparation: (Phenol case) Cumene hydroperoxide method, from diazonium salts. Reactions: Electrophilic substitution: Nitration, halogenation and sulphonation. Reimer-Tiemann Reaction, Gattermann-Koch Reaction, Houben-Hoesch Condensation, Schotten-Baumann Reaction.

Ethers (aliphatic and aromatic): Introduction, synthesis and reactions of ethers

Unit-V: Aldehydes and ketones

(Formaldehye, acetaldehyde, acetone and benzaldehyde)

Preparation: from acid chlorides and from nitriles. Reactions: Reaction with HCN, ROH, NaHSO₃, NH₂-G derivatives. Aldol Condensation, Cannizzaro's reaction, Wittig reaction, Benzoin condensation, Clemensen reduction and Wolff Kishner reduction, Meerwein-Pondorff Verley reduction, Analysis of aldehydes and ketones: haloform test, 2,4-DNP test, Tollens and Fehling test

- 1. T. W. Graham Solomons: Organic Chemistry, John Wiley and Sons.
- 2. Peter Sykes: A Guide Book to Mechanism in Organic Chemistry, Orient Longman.
- 3. I.L. Finar: Organic Chemistry (Vol. I & II), E. L. B. S.
- 4. R. T. Morrison & R. N. Boyd: Organic Chemistry, Prentice Hall.
- 5. G. W. Castellan: Physical Chemistry 4th Edn. Narosa (2004).
- 6. Rajaram: Thermodynamics.
- 7. Puri and Sharma: Text Book of Physical Chemistry.
- 8. Puri, Sharma and Pathania: Text Book of Physical Chemistry.
- 9. Gurdeep Raj: Advanced Physical Chemistry.

IPCH-2.4T: ANATOMY AND PHYSIOLOGY

(Units: 5, Hours: 60, Credits: 4)

Unit-I: Blood, Lymphatic and Skeletal system

Blood: Composition and functions of blood, RBC, WBC, platelets, homeostasis, blood groups, mechanism of clotting, Introduction to disorders of blood; **Lymphatic System:** Composition, formation and circulation of lymph, Spleen and its functions; **Skeletal System:** Structure and function of skeleton, Articulation and movement, Disorders of bones and joints.

Unit-II: GIT, Respiratory System and Sensory Organs

Gastrointestinal tract: Structure of the gastrointestinal tract, functions of its different parts including those of liver, pancreas and gall bladder, various gastrointestinal structures and their role in the digestion and absorption of food; **Respiratory System:** Structure of respiratory organs, functions of respiration mechanism and regulation of respiration, respiratory volumes and vital capacity; **Sensory Organs:** Structure and physiology of eye (vision), ear (hearing), taste buds, nose (smell) and skin.

Unit-III: Nervous System

Autonomic Nervous System: Physiology and functions of the autonomic nervous system, Mechanism of neurohumoral transmission in ANS; **Central Nervous System:** Functions of different parts of brain and spinal cord, Neurohumoral transmission in the central nervous system, reflex action, electroencephalogram, specialized functions of the brain, cranial nerves and their functions

Unit-IV: Urinary and Cardiovascular Systems

Urinary System: Structure and functions of the kidney and urinary tract, physiology of urine formation and acid base balance, brief introduction to disorders of kidney; **Cardio Vascular System:** Anatomy of heart and blood vessels, physiology of blood circulation, cardiac cycle, conducting system of heart, heart sound, electrocardiogram, blood pressure and its regulation.

Unit-V: Endocrine and Reproductive Systems

Endocrine Glands: Basic anatomy and physiology of pituitary, thyroid, parathyroid, adrenal glands and pancreas, local hormones, brief introduction to disorders of various endocrine glands; **Reproductive System:** Structure and functions of male and female reproductive system, sex hormones, physiology of menstrual cycle, and various stages of pregnancy and parturition.

- 1. Vander, Sherman and Luciano: Human Physiology, the Mechanism of Body Function.
- 2. John B. West: Best and Taylor's Physiological Basis of Medical Practice.
- 3. Gerard J. Tortora & Bryan Derikson: Principles of Anatomy and Physiology.
- 4. Arthur C. Guyton and John E. Hall: Text Book of Medical Physiology, Elsevier India.
- 5. Anne Waugh Allison Grant Ross and Wilson, Churchill Livingstone: Anatomy and Physiology in Health and Illness, Elsevier Publishers.

IPCH-2.5T: BIOCHEMISTRY (Units: 5, Hours: 60, Credits: 4)

Unit-I: Carbohydrates

Classification, general properties and biological importance of carbohydrates; Monosaccharides: Fischer and Haworth projections (open chain and cyclic structure) and stereoisomerism of Glucose and Fructose; Determination of configuration of monosaccharides, absolute configuration of Glucose and Fructose, Mutarotation, Disaccharides: Glycosidic bond, Structure determination of Sucrose and structures of cellobiose, maltose and lactose; Polysaccharides: Structural polysaccharides-Cellulose, Chitin and Peptidoglycan, Storage polysaccharides: Starch, Glycogen and Inulin, Glycosamino glycanes, artificial sugars, Metabolism of carbohydrates: glycolysis, TCA, ETC, Glycogenesis, glycogenolysis, gluconeogenesis Hexose monophosphate shunt [HMP shunt]; Diseases associated with carbohydrate metabolism.

Unit-II: Amino Acids and Proteins

Classification and biological importance of proteins, Amino acids: Structures, isomerism, properties and classification; Structure of proteins, Ramachandran plot; Synthesis and sequencing of proteins; Protein databases; Denaturation & its effect on biological activity; Metabolism of amino acids: Transamination & deamination, decarboxylation, Urea cycle; Diseases associated with various proteins, Proteins as biomarkers and Drug targets, Protein extraction and its applications in food and drug industry.

Unit-III: Fatty Acids and Lipids

Classification and biological importance of lipids; Fatty acids: Structures, isomerism, properties and classification, Fats and oils, waxes; Triacyl glycerols, Phospholipids and Spingo lipids; Sterols; Steroids: adreno corticoids, testosterone, progesterone, estrogens; formation & biochemical significance of bile acids, bile salts, ketone bodies, prostaglandins, Biological membranes, Metabolism of fatty acids: beta oxidation; Diseases associated with lipid metabolism.

Unit-IV: Nucleic Acids

History and discovery of DNA and RNA; Chemical structure of DNA and RNA: Purine & pyrimidine bases, sugars, & phosphoric acid. Nucleosides & nucleotides, Watson-Crick double helix model of DNA, Conformation of DNA- primary, secondary, tertiary level; formation of nucleosome; structure of chromosome, karyotyping; alternate forms of DNA; DNA supercoiling, types of RNA; denaturation and renaturation of DNA; Synthesis and sequencing of DNA; Nucleic acid databases, replication of DNA, transcription, genetic code, translation, Mutations, Nucleic acids as drug targets

Unit-V: Enzymes

History, nomenclature and classification of enzymes; Properties of enzymes, role of co-factors and coenzymes; Mechanism of action of enzymes; Kinetics of enzymes, double reciprocal plot, Km and Vmax; factors effecting enzymatic action; Enzyme inhibition. Enzymes as targets of drugs, enzymes from natural sources and their application

- 1. Donald Voet and Judith G. Voet: Biochemistry.
- 2. Albert L. Lehninger: Biochemistry.
- 3. Reginald H. Garret and Charles M. Grisham: Biochemistry.

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- 4. Stryer: Biochemistry.
- 5. U. Satyanarayana: Biochemistry.
- 6. Karp: Cell and Molecular Biology.
- 7. Cooper: Cell and Molecular Biology
- 8. Rasthogi: Cell and Molecular Biology
- Snustad Simmonds: Genetics.
- 10. Brooker: Genetics.

IPCH-2.3LAB: PHYSICAL AND ORGANIC CHEMISTRY LAB (Credits: 2, 3hrs/week)

Section A: Physical Chemistry

Thermochemistry

- 1. Determination of heat capacity of calorimeter for different volumes
- 2. Determination of enthalpy of neutralization of hydrochloric acid with sodium hydroxide
- 3. Determination of enthalpy of neutralization of acetic acid with ammonium hydroxide
- 4. Determination of enthalpy of ionization of acetic acid
- 5. Determination of integral enthalpy of solution of salts (KNO₃, NH₄Cl)
- 6. Determination of enthalpy of hydration of copper sulphate

Section B: Organic Chemistry

Preparations:

- (a) Bromination of Phenol/Aniline
- (b) Benzoylation of amines/phenols
- (c) Oxime and 2,4-dinitrophenylhydrazone of aldehyde/ketone

The following methods are to be applied in the preparation of the above mentioned compounds:

Purification: by crystallization/distillation

Purity check: by determination of melting point/boiling points and by TLC

Calculations: quantitative yields

- 1. A.I. Vogel: Textbook of Practical Organic Chemistry, 5th edition, Prentice-Hall.
- 2. F. G. Mann & B. C. Saunders: Practical Organic Chemistry, Orient Longman (1960).
- 3. B. D. Khosla, V. C. Garg and Gulati: Senior Practical Physical Chemistry, R. Chand & Co.
- 4. Alexander Findlay: Practical Physical Chemistry.
- 5. B. P. Levitt: Findlay's Practical Physical Chemistry.
- 6. P. S. Sindhu: Practicals in Physical Chemistry, A Modern Approach.

IPCH-2.4 LAB: ANATOMY AND PHYSIOLOGY LAB (Credits: 2, 3hrs/week)

- 1. Microscopic study of different tissues
- 2. Identification of bones and joints
- 3. Study of different systems with the help of charts and models
- 4. Estimation of RBC
- 5. Estimation of WBC
- 6. Estimation of haemoglobin
- 7. Different leukocyte count
- 8. Estimation of erythrocyte sedimentation rate
- 9. Determination of blood group
- 10. Determination of bleeding time
- 11. Determination of clotting time
- 12. Recording of human heart rate and pulse rate
- 13. Study of effect of posture and exercise on blood pressure
- 14. Recording human body temperature

- 1. Shukant R. Apte: Experimental Physiology.
- 2. Ramesh K. Goyal, Natyar M. Patel and Shailesh A. Shah: Practical Anatomy, Physiology and Biochemistry.
- 3. Sir John Y. Dacie and S. M. Lewis: Practical Haematology.

IPCH-2.5LAB: BIOCHEMISTRY LAB (Credits: 2, 3hrs/week)

- 1. Extraction of starch from Potato and its identification
- 2. Qualitative analysis of sugars
- 3. Qualitative analysis of Amino acids
- 4. Qualitative analysis of Lipids
- 5. Quantitative estimation of sugars by Anthrone method
- 6. Quantitative estimation of proteins by Biuret method
- 7. Extraction of DNA from Bacteria/Blood
- 8. Estimation of DNA by DPA method
- 9. Estimation of RNA by Orcinol method
- 10. Extraction of Amylase and determination of its activity
- 11. Separation and identification of amino acids by chromatography
- 12. Extraction of Casein from milk
- 13. Visualization of primary, secondary, tertiary structure of various proteins in PDB
- 14. Determination of blood glucose levels
- 15. Determination of SGOT and SGPT levels

- 1. Deshpandey and Shashidhar: Lab Manual.
- 2. Plummer: Lab Manual.
- 3. Sahney: Biochemistry Lab Manual.

SEMESTER-III

IPCH-3.2T: ENVIRONMENTAL SCIENCE

(Units: 5, Hours: 60, Credits: 4)

Unit-I: Earth's Spheres and Environmental Pollution

Structure of earth spheres, basics of bio-geochemical cycles, types of environmental pollution

Air Pollution: Types and sources, green house effect and global warming, measures for reversion of green house effect, acid rain, ozone depletion and their consequences on environment, photochemical smog, hazards related to power plants, chemical and biological warfare systems, strategies for air pollution control

Water Pollution: Hydrological cycle, types and sources of water pollution, composition of organic and inorganic water pollutants, ground water pollution, surface water pollution (lake and river water), marine pollution, mercury pollution, eutrophication, biodegradability of detergents and pesticides-case studies, harmful effects of water pollution and control strategies

Unit-II: Water Analysis and Waste Water Treatment

Water Analysis: Water quality criteria for domestic use (BIS), analysis of temperature, color, odor, taste, turbidity, pH (physical parameters), TDS, total alkalinity, hardness, Cl^- , F^- , residual-Cl, NH_3 , NO_3^- , NO_2^- , SO_4^{-2} , CO_3^{-2} , Na, K, Mg and Ca (chemical parameters), heavy metals, microbiological and pesticide residues

Water Treatment: Principles of water and waste water treatment for drinking and industrial use-(i) physical process (ii) biological process (iii) chemical processes - principles of coagulation, flocculation, softening, disinfection, electro-dialysis, reverse osmosis, demineralization, advanced oxidation process (AOP) and fluoridation

Dissolved oxygen (DO) and water aeration, chemical oxygen demand (COD), biochemical oxygen demand (BOD), aerobic and anaerobic treatment of waste water, aeration of water, activated sludge

Unit-III: Solid and Hazardous Waste Management

Solid Wastes: Soil fertility and solid wastes definition, types, sources, characteristics, and impact of solid wastes on environmental health

Solid-waste collection, segregation, transport and handling of wastes at source,

Solid waste processing technologies; chemical, physical and biological treatment for energy and other resource recovery-recycling and reuse,

Bio-remediation, composting and vermicomposting, Landfill design for sanitary and hazardous wastes and incineration, landfill bioreactors

Hazardous Wastes: Definition, categorization, sources and characteristics, hazardous waste collection, transport, treatment and disposal, legislation on management and handling of solid and hazardous wastes, disposal of medical and pharmaceutical waste.

Unit-IV: Energy Resources and Maintenance

Renewable and non-renewable energy resources, physico-chemical characteristics and energy content of coal, petroleum and natural gas, basic concept of various renewable energy resources and utilization-solar radiation and its spectral characteristics, solar energy for chemical synthesis, photovoltaics, wind energy, geothermal energy, ocean energy, hydroelectric energy, biomass energy & biofuels, hydrogen energy, cryogenic fuels, fuel-cells, energy storage and usage pattern, role of IT (information technology) in energy management, future energy need projection in India.

Environmental protection act; air, water, wild life and forest conservation act, basic concepts of biodiversity and biodiversity act.

Unit-V: Nuclear and Radiochemistry

Introduction, radioactive decay and equilibrium, types of nuclear reactions, nuclear fission and nuclear reactors, nuclear fusion, nuclear power plants and fuel production

Sources of radioactive pollution, biological effects, radiation detection, nuclear fallout and disasters examples, control of radiation/disposal options, basics of radiochemical separation, basics of tracer applications, radio carbon dating

Concept of environmental management and disaster reduction

- 1. Bureau of Indian Standards (BIS) IS:10500:2012, Drinking Water Specification, 2012
- 1. A. K. De: Environmental Pollution
- 2. Wark and Werner: Air Pollution
- 3. B. K. Sharma & H. Kaur: Environmental Pollution
- 4. P. K. Trivedi: Introduction to Air Pollution
- 5. D. D. Tyagi and M. Mehre: A Text Book of Environmental Pollution
- 6. C. S. Rao: Environmental Pollution Engineering and Control
- 7. Satake and M. Midu: Chemical in the Environment
- 8. G. Lunn and E. B. Sansone: Destruction of hazardous chemicals in the laboratory
- 9. A. E. Greenberg and A. D. Eaton: Standard Methods for Examination of Water and Waste Water, APHA, AWWA, WEF
- 10. D. S. Ramteke and C. A. Moghe: Manual on Water and Waste water analysis, NEERI
- 11. H. Kaur, Environmental Chemistry, 6th Edn, Pragathi Prakashan, Meerut, 2011
- 12. K. H. Mancy and W. J. Weber Jr: Analysis of Industrial Waste Water, Wiley Interescience, New York, 1971

PCH-3.3T: SOLUTIONS, ELECTROCHEMISTRY & FUNCTIONAL GROUP ORGANIC CHEMISTRY

(Units: 5, Hours: 60, Credits: 4)

Unit-I: Solutions and Phase Rule

Solutions: Liquid-liquid mixtures, ideal liquid mixtures, Raoult's and Henry's laws; Non-ideal systems; Azeotropes HCl-H2O and C2H5OH-H2O systems; Fractional distillation, Partially miscible liquids- Phenol-Water, Triethyl amine-Water and Nicotine-Water systems; Lower upper consolute temperatures; Effect of impurity on consolute temperature; Immiscible liquids and steam distillation

Phase Rule: Statement and meaning of the terms-Phase, Component and degrees of freedom, Gibb's Phase rule, phase equilibria of one component system-water system. Phase equilibria of two-component system-Solid-Liquid equilibria, simple eutectic Pb-Ag system, desilverisation of lead. Solid solutions- compound with congruent melting point Mg-Zn system and incongruent melting point NaCl-H₂O system

Unit-II: Electrochemistry

Electrical transport-conduction in metals and in electrolyte solutions, Specific conductance, Equivalent conductance and molecular conductance, measurement of equivalent conductance, variation of specific conductance and equivalent conductance with dilution; Migration of ions-Relative speed of ions during electrolysis; Transport Number-definition and determination by Hittorf's method for attackable and unattackable electrodes; Kohlraush law of independent migration of ions and applications; Theory of electrolyte dissociation and its limitations, weak and strong electrolytes, Ostwald's dilution law-its uses and limitations; Debye-Huckel theory of strong electrolytes, Debye-Huckel-Onsager equation for strong electrolytes (elementary treatment only)

Difference between electrolytic cell and Galvanic cell; Galvanic cells- Conventional cell representation of Galvanic cells, Single electrode potential, Standard electrode potential

EMF of a cell and its measurement, reference electrodes-Standard hydrogen electrode (SHE) and Calomel electrode; Electrode reactions-Nernst equation; Reversible and Irreversible cells, Types of reversible electrodes-gas electrode, metal-metal ion electrode, metal-metal insoluble salt electrode and redox electrodes; Calculation of thermodynamic quantities of cell reactions (ΔG , ΔH and K)

Unit-III: Carboxylic acids, Amines and Their Derivatives

Carboxylic acids (aliphatic and aromatic)

Preparation and reactions including Hell-Vohlard-Zelinsky Reaction

Carboxylic acid derivatives (aliphatic):

Preparation: Acid chlorides, Anhydrides, Esters and Amides from acids and their interconversion.

Reactions: Comparative study of nucleophilicity of acyl derivatives. Reformatsky Reaction, Perkin condensation.

Amines and Diazonium Salts

Amines (Aliphatic and Aromatic):

Preparation: from alkyl halides, Gabriel's Phthalimide synthesis, Hofmann Bromamide reaction.

Reactions: Hofmann vs. Saytzeff elimination, Quaternary ammonium salts, Carbylamine test, Hinsberg test, test with HNO₂, Schotten-Baumann Reaction. Electrophilic substitution (case aniline): nitration, bromination, sulphonation.

Diazonium salts: Preparation: from aromatic amines.

Reactions: conversion to benzene, phenol, dyes.

Unit-IV: Amino Acids and Peptides

Preparation of Amino Acids: Strecker synthesis using Gabriel's phthalimide synthesis. Zwitterion, Isoelectric point and Electrophoresis

Reactions of Amino acids: ester of –COOH group, acetylation of –NH₂ group, complexation with Cu²⁺ ions, ninhydrin test.

Determination of Primary structure of Peptides by degradation Edmann degradation (N-terminal) and C-terminal (thiohydantoin and with carboxypeptidase enzyme); Synthesis of simple peptides (up to dipeptides) using coupling reagents (EDC/HOBt, DCC, DIC, HATU) and discuss the advantages of various coupling reagents

Unit-V: Nitro Compounds

Classification, Tautomerism of nitroalkanes (nitro form and aci form), Preparation (nitroalkanes and alkyl nitrites), Reactivity: Halogenation using nitrous acid, Nef reaction, Michael Addition, Henry Reaction, Aromatic Nitro hydrocarbons, Preparation of Nitrobenzene from diazonium salt and direct nitration, Reactivity and reduction of nitrobenzene in different media

- 1. Mahan, B. H: University Chemistry, 3rd Ed. Narosa (1998).
- 2. Petrucci, R. H: General Chemistry, 5th Edn, Macmillan Publishing Co.: New York (1985).
- 3. Morrison, R. T. & Boyd, R. N: Organic Chemistry, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- 4. Finar, I. L: Organic Chemistry (vol.1), Dorling Kindersley (India) Pvt. Ltd. (Pearson Edn).
- 5. Finar, I. L: Organic Chemistry (vol.2), Dorling Kindersley (India) Pvt. Ltd. (Pearson Edn).
- 6. Nelson, D. L & Cox, M. M: Lehninger's Principles of Biochemistry, 7th Edn, W. H. Freeman.
- 7. Berg, J. M., Tymoczko, J. L. & Stryer, L. Biochemistry, W.H. Freeman (2002).
- 8. Prutton and Marron: Principles of Physical Chemistry.
- 9. Puri and Sharma: Text Book of Physical Chemistry.
- 10. S. K. Dogra: Physical Chemistry Through Problems.
- 11. Puri, Sharma and Pathania: Text Book of Physical Chemistry
- 12. Gurdeep Raj: Advanced Physical Chemistry

IPCH-3.4T: PHARMACEUTICAL ANALYSIS

(Units: 5, Hours: 60, Credits: 4)

Unit-I: Fundamentals of Chemical Analysis

Introduction to analytical chemistry and chemical analysis, applications of chemical analysis, review of basic chemical measurements, units, and concentrations, types of analysis, classifications of analytical techniques based on sample and methods of analysis, factors affecting the choice of analytical methods, sampling, sampling procedures, principles of sample preparation, including digestion, precipitation, extraction (including solvent extraction, ion pair extraction, solid phase extraction), fusion, ashing, drying, hazards in sampling, accuracy, precision, calibration, errors, types of errors, propagation of errors, minimization of errors

Unit-II: Volumetric Analysis-I

Theoretical considerations and pharmaceutical applications with special reference to Indian Pharmacopoeia of the following analytical techniques

Acid-Base titrations: primary and secondary standards, Law of mass action, hydrolysis of salts, neutralization curves, and theory of indicators, choice of indicators, mixed indicator, application in assay of Benzoic acid, Boric acid, Aspirin as per IP.

Non-Aqueous titrations: Types of solvents, end point detection, application in assay of Sodium acetate, Sodium benzoate, Norfloxacin tablet as per IP

Oxidation-Reduction titrations: Theory of redox titration, oxidation-reduction curves, redox Indicators, pharmaceutical applications, preparation and standardization of redox titrants like potassium permanganate, ceric ammonium sulphate, sodium thiosulphate, titanous chloride, applications in assay of Ferrous sulfate, Ascorbic acid, Isoniazide, Hydrogen peroxide, Iodine (Iodimetry and Iodometry)

Unit-III: Volumetric Analysis-II

Theoretical considerations and pharmaceutical applications with special reference to Indian Pharmacopoeia of the following analytical techniques

Complexometric Titrations: Formation of complex and its stability, methods to increase the selectivity of EDTA titrations, titration curves, metallochrome indicators, types of EDTA titrations, application in assay of Magnesium sulfate, Lead nitrate and calcium gluconate.

Argentometric Titrations: theory of precipitation, factors affecting solubility of a precipitate, titration methods Mohr's, Volhard's, Gay lussac, and Fajan's method, indicators. Applications in assay of Potassium chloride, Sodium chloride and Ammonium chloride

Unit-IV: Chromatography

Principles and classification with relevant examples of pharmaceutical products involving separation of drugs from excipients or impurities using following chromatographic techniques

TLC: Introduction, principle, techniques, Rf value, resolution, mobile and stationary phases, applications and visualization methods

Column Chromatography: Adsorption column chromatography, Operational technique, frontal analysis and elution analysis. Factors affecting column efficiency, applications

HPLC: Instrumentation, types of Columns and Detectors; its applications

Unit-V: Spectroscopic Techniques

Introduction to theory of electronic, atomic and molecular spectra, Fundamental laws of photometry, Beer-Lambert's Law, application and its deviation, limitation of Beer law, application of the law to

single and multiple component analysis, Spectra of isolated chromophores, auxochromes, bathochromic shift, hyperchromic and hypochromic effect, effect of solvent on absorption spectra, molecular structure, Photometer, U.V-Visible spectrophotometer-sources of U.V-Visible radiations, collimating systems, monochromators, samples cells and following detectors-Photocell, Barrier layer cell, Phototube, Diode array, applications of U.V-Visible spectroscopy in pharmacy and spectrophotometric titrations with examples from IP.

- 1. Gary D. Christian: Analytical Chemistry, 6th edition, John Wiley & sons Inc.
- 2. Douglas A. Skoog, Donald M. West, James F. Holler, Stanley R. Crouch: Fundamentals of Analytical Chemistry.
- 3. Banwell and McCash: Fundamentals of Molecular Spectroscopy, 4th edn, Tata McGraw Hill
- 4. Day and Underwood: Quantitative Analysis, 6th Edition, PHI, 2009.
- 5. David Harvey: Modern Analytical Chemistry, McGraw Hill, 2000,
- 6. Chatwal K, Anand: Instrumental Methods of Chemical Analysis, 5th edition.
- 7. G. H. Jeffery, J. Bassett, J. Mendhan, R. C. Denny: Vogel's text book of Quantitative Chemical Analysis.
- 8. Willard, Merit, Dean, Settle: Instrumental Methods of Analysis.
- 9. Y. R. Sharma: Organic Spectroscopy.
- 10. Silverstein, Webster: Spectrometric Identification of Organic Compounds.
- 11. Henry P. Talbot: An introductory Course of Quantitative Chemical Analysis with Explanatory Notes, 6th edition.
- 12. Indian Pharmacopoeia, BP, USP.
- 13. Remington: The Science and Practice of Pharmacy, 20th edition.
- 14. Donald Cairns: Essentials of Pharmaceutical Chemistry, third edn, Pharmaceutical press.
- 15. A. H. Becket and J. B. Stenlake: Practical Pharmaceutical Chemistry, 4th edn, the Athlone press.

IPCH-3.5T: CELL AND MOLECULAR BIOLOGY (Units: 5, Hours: 60, Credits: 4)

Unit-I:

Cell organelles of Eukaryotic Cell: Dynamic structure of membrane and its function, Chemical composition of membrane-Membrane lipids, Proteins and carbohydrates; Membrane fluidity, Membrane transport-Passive and Active transport, Movement of ions through membrane-Ion Channels; Neurotransmission, Action of drugs on Synapses; Mitochondrial structure and function; Endoplasmic Reticulum; Golgi complex; Ribosomes; Peroxisomes; Extracellular matrix in Animal Cells, Interaction of Cells with Extracellular matrix, Interactions of Cells with other Cells

Unit-II:

Cell Cycle, Cell Cycles in Vivo, Regulation of Cell Cycle by cyclin dependent Kinases (CdKs); Mitosis, its stages and significance, Meiosis, its stages and significance, Gametogenesis, Mitotic and Meiotic nondisjunction and its consequences; Apoptosis, Extrinsic and Intrinsic Pathways of Apoptosis, Cancer, Properties of Cancer Cells, Different types of Cancers, Causes of Cancer, Genetics of cancer-Tumour-Suppressor genes and Oncogenes, Strategies for combating Cancer

Unit-III:

Signal Transduction-Cell signaling, Different types of Cell signaling systems, Signaling pathway; Extracellular messengers and their receptors, Secondary messengers and their role in Signal Transduction-c AMP, Inositol 1,4,5 triphosphate, Diacylglycerol and Calcium; Signal Transduction by G Protein Coupled Receptors and Receptors Protein-Tyrosine Kinases(RTKs) with suitable examples, Insulin Signaling defect in Diabetes mellitus

Unit-IV:

Gene as a unit of inheritance, Chromosome-Carriers of genes, Chromosome structure -centromere, Telomere, satelite DNA; Cytological techniques used to study chromosomes, Karyotype of Humans, Location of genes on chromosomes-Fluorescent insitu Hybridization; Separation of chromosomes-Fluorescent Activated Cell Sorter; Chromosomal aberrations: Structural aberrations- Inversion, Deletion, Duplication, Translation. Numerical abberations- Hypoploidy, Hyperploidy, Polyploidy; Diseases associated with chromosomal abnormalities (Autosomal/Sex chromosomal), Prenatal diagnosis of Chromosomal abnormalities

Unit-V:

The concept of Genome, Organization of genome in Virus &Bacteria, Genome organization and role of Histone proteins in Eukaryotes; The complexity of the genome -Denaturation & Renaturation, Reassociation Kinetics, Cot Curves, Human genome Project, Genetic variation within the human species population-1) DNA sequence variation, 2) Copy number variation, 3) Structural variation; Application of Genome analysis to Medicine, Amplification of Gene-Polymerase Chain Reaction, Primer designing; Molecular diagnosis of Diseases

- 1. Snustad Simmons: Principles of Genetics.
- 2. Daniel L. Hartl and Elizabeth W Jones: Genetics.
- 3. Robert J. Brooker: Genetics.
- 4. Peter J. Russell: Genetics.

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- 5. Gerald Karp and Nancy L Pruitt: Cell Molecular Biology.
- 6. Cooper: Cell and Molecular Biology.
- 7. David Baltimore and Harvey Lodish: Molecular Cell Biology. Peparinent of Phannaceutical Chemistry, It, Wills

IPCH-3.3LAB: PHYSICAL CHEMISTRY AND ORGANIC CHEMISTRY LAB (Credits: 2, 3hrs/week)

Physical Chemistry

Critical solution temperature (CST)

- 1. Determination of CST of phenol-water system
- 2. Effect of salt on the CST in phenol-water system

Distribution

- 1. Distribution of acetic acid between n-butanol and water
- 2. Distribution of benzoic acid between toluene and water

Conductance

- 1. Determination of Cell constant
- 2. Verification of Ostwald's dilution law using a weak acid
- 3. Conductometric titration of strong acid Vs strong base
- 4. Conductometric titration of weak acid Vs strong base
- 5. Conductometric titration of a mixture of strong acid and weak acid Vs strong base

Organic Chemistry

Systematic identification of organic compounds possessing mono functional groups (-COOH, phenolic, aldehydic, ketonic, amide, nitro, amines), preparation & purification of one derivative and detection of extra elements (N, S, Cl, Br, I) present in the above mentioned functional group containing organic compounds.

- 1. Vogel, A. I., Tatchell, A. R., Furnis, B. S., Hannaford, A. J. & Smith, P. W. G: Textbook of Practical Organic Chemistry, Prentice-Hall, 5th edition (1996).
- 2. Mann, F. G. & Saunders, B. C: Practical Organic Chemistry Orient-Longman (1960).
- 3. Khosla, B. D.; Garg, V. C. & Gulati, A: Senior Practical Physical Chemistry, R. Chand & Co.
- 4. Ahluwalia, V.K. & Aggarwal, R: Comprehensive Practical Organic Chemistry.
- 5. B. D. Khosla, V. C. Garg and Gulati: Senior Practical Physical Chemistry, R. Chand & Co.
- 6. Alexander Findlay: Practical Physical Chemistry.
- 7. B. P. Levitt: Findlay's Practical Physical Chemistry.
- 8. P. S. Sindhu: Practicals in Physical Chemistry, A Modern Approach.

IPCH-3.4LAB: PHARMACEUTICAL ANALYSIS LAB (Credits: 2, 3hrs/week)

All the experiments are to be repeated for at least three times and data generated for every experiment has to be entered in Microsoft excel file.

- 1. Determination of % purity of sodium benzoate.
- 2. Determination of λmax of KMnO₄
- 3. Determination of λ max of paracetamol
- 4. Preparation and standardization of iodine solution
- 5. Assay ferrous sulphate
- 6. Assay of norfloxacin tablets and chlorpromazine tablets
- 7. Experiment related to sampling of drugs from formulations
- 8. Experiment related to sampling of drugs from biological fluids
- 9. TLC profile of paracetamol and para aminophenol using various mobile phases
- 10. TLC profile of aspirin and salicylic acid using various mobile phases
- 11. Demonstration of column chromatography
- 12. Estimation of paracetamol using calibration curve method
- 13. Assay of paracetamol tablets and syrup
- 14. Estimation of effect of solvent, concentration on absorption of compounds
- 15. Demonstration of bathochromic shift and hypsochromic shift
- 16. Comparison of methods of assay of aspirin using titrimetry and spectroscopy

- 1. Gary D. Christian: Analytical Chemistry, 6th edition, John Wiley & sons Inc.
- 2. A. H. Becket and J. B. Stenlake: Practical Pharmaceutical Chemistry, 4th edn, the Athlone press
- 3. Henry P. Talbot: An introductory Course of Quantitative Chemical Analysis with Explanatory Notes, 6th edition.
- 4. G. H. Jeffery, J. Bassett, J. Mendhan, R. C. Denny: Vogel's text book of Quantitative Chemical Analysis.

IPCH-3.5LAB: CELL AND MOLECULAR BIOLOGY LAB (Credits: 2, 3hrs/week)

- 1. Isolation of Mitochondria
- 2. Dialysis
- 3. Study of Mitosis (and microscopic observation of mitotic phases)
- 4. Study of Meiosis
- 5. Human karyotype
- 6. Identification of chromosomal abnormalities from karyotype
- 7. Problems on Reassociation Kinetics
- 8. Primer designing for PCR
- 9. Amplification of genes by PCR

SEMESTER-IV

IPCH-4.2T: CHEMISTRY OF NUTRACEUTICALS AND DAIRY PRODUCTS (Units: 5, Hours: 60, Credits: 4)

Unit-I: Nutrients

Food as a source of nutrients, functions of food, definition of nutrients, food pyramid, energy yielding and protective nutrients

Carbohydrates: Sources, functions, storage in the body and utilization of carbohydrates

Proteins: Sources, functions, essential and non-essential amino acids

Lipids: Classification, sources and requirements, essential fatty acids, functions of triglycerides, phospholipids, lipoproteins and cholesterol

Vitamins: Classification, sources and requirements, effects of deficiency of vitamins

Minerals: Sources, functions, bioavailability, effects of deficiency of minerals

Unit-II: Nutraceuticals

Introduction to nutraceuticals, definitions, basis of claims for a compound as a nutraceutical, regulatory issues for nutraceuticals including CODEX; concept of angiogenesis and the role of nutraceuticals; nutraceuticals for management of various diseases; nutraceuticals and their mechanisms of action and dosage levels.

Unit-III: Manufacture of Nutraceuticals

Manufacturing aspects of selected nutraceuticals such as lycopene, isoflavonoids, prebiotics and probiotics, glucosamine, phytosterols; formulation of functional foods containing nutraceuticals-stability issues, analytical issues and labelling issues; clinical testing of nutraceuticals and health foods; adverse effects and toxicity of nutraceuticals.

Unit-IV: Analysis of Milk and Milk Products

Sampling of milk and milk products, Roese-Gottlich fat analysis, determination of specific gravity, total solid, acidity, sediment test, analysis of butter-modified Kohman test, detection of added water, total solid-Marshall rennet test, methylene blue test, Reazurin test, alcohol test, Arnold Guaiac test, Phosphatase test.

Unit-V: Production of Milk Products

Manufacture of condensed milk, milk powder, cheese, ice-cream, butter, ghee, malted products, evaporated and dried products, their evaluation and quality parameters, defects encountered during production, packaging and storage.

- 1. Swaminathan, M: Advanced Text Book on Food and Nutrition, Vol-I, BAPPCO Publishers, Bangalore (1985).
- 2. Swaminathan, M: Advanced Text Book on Food and Nutrition, Vol-II, BAPPCO Publishers, Bangalore (1985).
- 3. Srilaxmi, B: Nutrition Science, New Age International (p) Ltd Publishers (2003).
- 4. Geoffrey, P: Dietary Supplements and Functional Foods, Blackwell Publishing (2006).
- 5. Losso, J. N: Angi-angiogenic Functional and Medicinal Foods, CRC Press (2007).
- 6. Cupp, J and Tracy, T. S: Dietary Supplements: Toxicology and Clinical Pharmacology, Humana Press (2003).
- 7. Manson, P: Dietary Supplements (2nd Ed) Pharmaceutical Press (2001).

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- 8. Campbell, J. E and Summers, J. L: Dietary Supplement Labeling Compliance (2004).
- 9. Shi, J: Functional Food Ingredients and Nutraceuticals: Processing Technologies, Taylor & Francis Publ. CRC Press (2007).
- 10. Goldberg, I: Functional Foods: Designer Foods, Pharma foods, Nutraceuticals Chapman & Hall (1999).
- 11. Robert, E. C: Handbook of Nutraceuticals and Functional Foods, Wildman (2006).
- 12. Neeser, J. R and German, B. J: Bioprocesses and Biotechnology for Functional Foods and Nutraceuticals, Marcel Dekker (2004).
- 13. Milk and Milk Products, 4th Edn, Tata McGraw Hill Publishing Company Ltd, New Delhi (1973).
- 14. Jenness, R and Patton, S: Principles of Dairy Chemistry, John Wiley & Sons, New York
- 15. Webb, B. H; Johnson A. H and Alford J. A: Fundamentals of Dairy Chemistry, 2nd Edn, AVI, Westport, USA (1974).
- 16. Wong, N. P; Jenness, R; Kennedy, M and Marth, E. H: Fundamentals of Dairy Chemistry, 3rd Edn, Van Norstrand Reinhold, New York.

IPCH-4.3T: COORDINATION CHEMISTRY, CHEMICAL KINETICS, DILUTE SOLUTIONS & COLLIGATIVE PROPERTIES, COLLOIDS & SURFACE CHEMISTRY (Units: 5, Hours: 60, Credits: 4)

Unit-I: Transition Elements (3d series)

General group trends with special reference to electronic configuration, variable valency, colour, magnetic and catalytic properties, ability to form complexes and stability of various oxidation states (Latimer diagrams) for Mn, Fe and Cu.

Lanthanoids and Actinoids: Electronic configurations, oxidation states, colour, magnetic properties, lanthanide contraction, separation of lanthanides (ion exchange method only).

Transition metal organometallics as reagents in stoichiometric organic synthetic reactions (preliminary information)

Unit-II: Coordination Chemistry

Valence Bond Theory (VBT): IUPAC system of nomenclature, Inner and outer orbital complexes of Cr, Fe, Co, Ni and Cu (coordination numbers 4 and 6). Structural and stereoisomerism in complexes with coordination numbers 4 and 6. Drawbacks of VBT

Crystal Field Theory

Crystal field effect, splitting of d-orbital in octahedral geometry (regular, compressed and elongated), Crystal field stabilization energy (CFSE), Crystal field effects for weak and strong fields, Tetrahedral symmetry, Factors affecting the magnitude of D (10 DQ), Spectrochemical series, Comparison of CFSE for Oh and Td complexes, Tetragonal distortion of octahedral geometry. Jahn-Teller distortion, square planar coordination, d-orbital splitting in square pyramidal, trigonal bipyramidal and linear geometries; applications of CFT

Unit-III: Chemical Kinetics

Introduction to chemical kinetics, rate of reaction, variation of concentration with time, rate laws and rate constant; Specific reaction rate, Factors influencing reaction rates: effect of concentration of reactants, effect of temperature, effect of pressure, effect of surface area of reactants, effect of radiation, effect of catalyst with simple examples, order of reaction. First order reaction, derivation of equation for rate constant; Characteristics of first order reaction. Units for rate constant; Half- life period, graph of first order reaction examples-decomposition of H2O2; Pseudo first order reaction examples-hydrolysis of methyl acetate, inversion of cane sugar, problems. Second order reaction, derivation of expression for 2nd order rate constant, examples-saponification of ester. Characteristics of second order reaction, units for rate constants, half- life period and second order plots. Zero order reaction: derivation of rate expression, examples i)combination of H2 and Cl2 to form HCl, ii) thermal decomposition of HI on gold surface characteristics of Zero order reaction units of k, half-life period and graph, problems

Methods of determination of order of reaction: i) method of integration, ii) half life method, iii) van't-Hoff differential method iv) Ostwald's isolation method. Problems

Effect of temperature on reaction rate: Arrhenius equation, temperature coefficient, concept of energy of activation, determination of energy of activation from Arrhenius equation and by graphical method, problems; Simple collision theory based on hard sphere model, explanation of frequency factor, orientation or steric factor

Unit-IV: Dilute Solutions and Colligative Properties

Dilute Solutions, Colligative Properties, Raoult's law, relative lowering of vapour pressure, molecular weight determination. Osmosis - laws of osmotic pressure, its measurement, determination of molecular weight from osmotic pressure; Elevation of boiling point and depression of freezing point; Derivation of relation between molecular weight and elevation in boiling point and depression in freezing point; Experimental methods for determining various colligative properties; Abnormal molar mass, Van't hoff factor, degree of dissociation and association of solutes

Unit-V: Colloids and Surface Chemistry

Definition of colloids, Classification of colloids; Solids in liquids (sols): preparations and properties-(including Kinetic, Optical and Electrical stability of colloids) Protective action. Hardy-Schultz law, Gold number; Liquids in liquids (emulsions): Types of emulsions, preparation and emulsifier. Liquids in solids (gels); Classification, preparations and properties, General applications of colloid; Micelles: Classification of surface active agents; Surfactant action, micellization and micellar interactions, Structure of micelles – spherical and laminar; Critical micellar concentration (CMC). Factors affecting the CMC of surfactants; Counter ion binding to micelles

Adsorption: Types of adsorption, Factors influencing adsorption; Freundlich adsorption isotherm; Langmuir theory of unilayer adsorption isotherm; applications

- 1. Kotz, J. C., Treichel, P. M. & Townsend, J. R: General Chemistry Cengage Learning India Pvt. Ltd., New Delhi (2009).
- 2. Mahan, B. H: University Chemistry, 3rd Ed. Narosa (1998).
- 3. Petrucci, R. H: General Chemistry, 5th Ed. Macmillan Publishing Co.: New York (1985).
- 4. Cotton, F. A. & Wilkinson, G: Basic Inorganic Chemistry, Wiley.
- 5. Shriver, D. F. & Atkins, P. W: Inorganic Chemistry, Oxford University Press.
- 6. Wulfsberg, G: Inorganic Chemistry, Viva Books Pvt. Ltd.
- 7. Rodgers, G. E: Inorganic & Solid State Chemistry, Cengage Learning India Ltd (2008).
- 8. G. M. Barrow: Physical Chemistry Tata McGraw-Hill (2007).
- 9. G. W. Castellan: Physical Chemistry 4th Edn. Narosa (2004).
- 10. Prutton and Marron: Principles of Physical Chemistry.
- 11. Puri and Sharma: Text Book of Physical Chemistry.
- 12. S. K. Dogra: Physical Chemistry through Problems.
- 13. Lewis and Glasstone: Elements of Physical Chemistry.
- 14. Atkins: Physical Chemistry.
- 15. Puri, Sharma and Pathania: Text Book of Physical Chemistry.
- 16. Gurdeep Raj: Advanced Physical Chemistry.

IPCH-4.4T: PHARMACOLOY-1 (Units: 5, Hours: 60, Credits: 4)

Pharmacology-1 (Basics of Pharmacokinetics and Pharmacodynamics)

Note: The following units are essential to a pharmaceutical chemist to understand and design new molecules.

Unit-I: Drug Action at Receptors

Structure and classification of receptors, general mode of operation, Superfamily Type 1, 2, 3, 4, Ligand–receptor relationships, The chemical nature of the binding of ligands to receptors, Neurotransmitters, signaling process, Ion channels and their control, Membrane-bound enzymes-activation/deactivation, conformational changes in receptor, Binding groups, Position of binding, Size and shape, ligand concentration–response curves (Agonist concentration–response relationships, Antagonist concentration–receptor relationships), Ligand-receptor theories (Clark's occupancy theory, rate theory, two-state model), Citalopram, an antagonist antidepressant –case study, □-Blockers

Unit-II: ADME

Scheme of fate of dosage form after its administration, definition and introduction to concept of absorption, distribution, biotransformation and elimination of drug, Introduction to bioavailability and various equivalence referring plasma time profile of drug, significance of metabolisms involved in the absorption and bio transformation of drugs, effects of physico-chemical, pharmaceutical and biological factors on ADME, renal and non-renal excretion, Concept of clearance, disintegration and dissolution studies

Unit-III: Barriers to Drug Exposure in Living Systems

Introduction to Barriers, drug dosing, barriers in the mouth, stomach, gastrointestinal tract, kidney, permeation of the gastrointestinal cellular membrane, metabolism in the Intestine, enzymatic hydrolysis in the intestine, absorption enhancement in the Intestine, barriers in the blood stream, plasma enzyme hydrolysis, plasma protein binding, red blood cell binding, blood brain barrier,

Unit-IV: Plasma Membrane

The plasma membrane (Lipid, protein, carbohydrate components), Similarities and differences between plasma membranes in different cells, Cell walls, Bacterial cell and animal cell exterior surfaces, Virus, Tissue, Human skin, The transfer of species through cell membranes, (Osmosis, Filtration, Passive diffusion, Facilitated diffusion, Active transport, Endocytosis, Exocytosis), examples of drugs that affects the structure of cell membranes and walls (anti-infective agents, Local anaesthetics)

Unit-V: Chemotherapy

General principle of chemotherapy (various targets of chemotherapy covering pathology of infection and mechanism of actions of drugs, concept of resistance), Sulphonamides and co-trimoxazole, Antibiotics-Penicillins, Cephalosporins, Chloramphenicol, Macrolides, Quinolines and Fluoroquinolins, Quinolones, Tetracyclines, Aminoglycosides and miscellaneous antibiotics; Chemotherapy of tuberculosis, leprosy, fungal diseases, viral diseases, AIDS, protozoal diseases, worm infections, urinary tract infections and sexually transmitted diseases.

- 1. Graham L. Patrick: An Introduction to Medicinal Chemistry, Oxford University Press.
- 2. Gareth Thomas: Medicinal Chemistry, 2nd edition, John Wiley & Sons Ltd.
- 3. Donald Cairns: Essentials of Pharmaceutical Chemistry, third edn, Pharmaceutical Press.
- 4. Edward H. Kerns and Li Di: Drug Like Properties: Concepts, Structure Design and Methods: from ADME to Toxicity Optimization, Elsevier Publications.
- 5. Bertram G. Katzung (International edition): Basic and Clinical pharmacology, Lange Medical Book / Mc Graw Hill, USA 2001 8th edition.
- 6. Rang H. P, Dale M.M and Ritter J.M, Churchill Livingston: Pharmacology, London, 4th edn
- 7. Goodman and Gilman's the Pharmacological Basis of Therapeutics (International edition) Mc Graw Hill, USA 2001 10th edition.
- 8. Braunwald, Fauci, Kasper, Hauser and Longo Jameson: Harrison's Principles of Internal Medicine (two volumes), 2001, Mc Graw Hill, New York, 15th edition.
- 9. H. Gerhard Vogel: Drug Discovery and Evaluation-Pharmacological Assays, 2nd edition, Springer Verlag, Berlin, Heidelberg.
- 10. A. H. Becket and J. B. Stenlake: Practical Pharmaceutical Chemistry, 4th edition, the Athlone press.
- 11. Sara E. Rosenbaum: Basic Pharmacokinetics and Pharmacodynamics: An Integrated Text Book and Computer Simulations, Wiley publications.

IPCH-4.5T: GENETIC ENGINEERING AND ITS APPLICATIONS IN PHARMACEUTICAL SCIENCES

(Units: 5, Hours: 60, Credits: 4)

Unit-I:

Concept of Genetic Engineering, Formulation of a recombinant protein production, Enzymes used in Gene Cloning-Restriction Endonucleases and their role in Gene Cloning, Nucleases, Ligases, Polymerases and DNA modifying enzymes; Characteristic features of Plasmids, Development of Vectors, Cloning and Expression vectors, Plasmid Vectors, Bacteriophage vectors, Cosmids, Phasmids, M-13 vectors Phagemids, Yeast vectors

Unit-II:

Construction of Genomic and c-DNA libraries, Labelling of Nucleic acids and antibodies (probes), Screening DNA Libraries for the desired clone- 1) Direct selection for the desired clone- Genetic selection 2) Identification of the clone from a gene library -Colony/ Plaque hybridization; Detection of Genes and Gene products- Southern Blotting, Northern Blotting, Western Blotting; Applications of Genetic Engineering- Production of recombinant hormones and vaccines by Genetically Engineered Microorganisms

Unit-III:

Laboratory requirements for Animal Cell Culture, Media designing, Types of media, Selection of media, Preparation, Sterilization of glassware, apparatus, reagents and media; Primary Cell Culture, Secondary Cell Culture; Disaggregation of tissues; Cell lines, Selection, maintenance and preservation of cell lines; Stem cell isolation, culture and application; Cell hybridization technology, Production of Monoclonal antibodies by Hybridoma Technology, application of Monoclonal antibodies in Pharmaceutical Sciences

Unit-IV:

Development of Transgenic Animals, Methods of DNA delivary-Microinjection, Calcium phosphate precipitation, Transformation with polyplexes, Transformation with liposomes and lipoplexes, Electroporation; Transgenic Mice technology, Molecular pharming-Production of Pharmaceutical products by Transgenic Animals, their (extraction and purification); Gene therapy: in-vivo and ex-vivo gene therapy with suitable examples

Unit-V:

Laboratory requirements for Plant Tissue Culture; MS media, Media sterilization, explant sterilization; Callus induction and its culture, Suspension culture; Micropropagation of pharmaceutically important plants; Production of Pharmaceutical products by Plant Tissue Culture, Development of Transgenic plants, Gene transfer to Plant Cells-Agrobacterium mediated transformation, Protoplast transformation, Particle bombardment; Transgenic Plants- Bt-Cotton, Transgenic Tomato-Flavr-Savor, Golden Rice

- 1. S. B. Primrose and R. M. Twyman: Principles of Gene Manipulation and Genomics.
- 2. T. A Brown: Gene Cloning and DNA Analysis.
- 3. Glick and Pasternak: Molecular Biotechnology: Principles and Applications.
- 4. Pratik Satya: Genomics and Genetic Engineering.
- 5. A. J Nair: Introduction to Biotechnology and Genetic Engineering.

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- 6. Ian Freshney: Culture of Animal Cells.
- 7. Tom Strachen and A P Read: Human Molecular Genetics.
- 8. H. K. Das: Biotechnology.
- 9. S. S. Bhojwaninand and A. Razdan: Plant Tissue Culture

IPCH-4.3LAB: INORGANIC AND PHYSICAL CHEMISTRY LAB (Credits: 2, 3hrs/week)

Inorganic Chemistry

Semi-micro qualitative analysis using H₂S of mixtures - not more than four ionic species (two anions and two cations and excluding insoluble salts) out of the following:

Cations: NH_4^+ , Pb^{2+} , Ag^+ , Bi^{3+} , Cu^{2+} , Cd^{2+} , Sn^{2+} , Fe^{3+} , Al^{3+} , Co^{2+} , Cr^{3+} , Ni^{2+} , Mn^{2+} , Zn^{2+} , Ba^{2+} , Sr^{2+} , Ca^{2+} , K^+

Anions: CO_3^{2-} , S^{2-} , SO^{2-} , $S_2O_3^{2-}$, NO_3^{-} , CH_3COO^- , CI^- , Br^- , I^- , NO_3^- , SO_4^{2-} , PO_4^{3-} , BO_3^{3-} , $C_2O_4^{2-}$, F^- (Spot tests should be carried out wherever feasible)

1) Estimate the amount of nickel present in a given solution as bis(dimethylglyoximato) nickel(II) or aluminium as oximate in a given solution gravimetrically. 2) Draw calibration curve (absorbance at λ_{max} vs. concentration) for various concentrations of a given coloured compound (KMnO₄/CuSO₄) and estimate the concentration of the same in a given solution. 3) Determine the composition of the Fe³⁺-salicylic acid complex solution by Job's method; 4) Estimation of (i) Mg²⁺ or (ii) Zn²⁺ by complexometric titrations using EDTA; 5) Estimation of total hardness of a given sample of water by complexometric titration. 6) Determination of concentration of Na⁺ and K⁺ using Flame Photometry.

Physical Chemistry

Adsorption

1. Adsorption of acetic acid on animal charcoal, verification of Freundlich isotherm.

Colloidal Solution

1. Preparation of sol solution of arsenic sulphide and estimation of flocculation value for NaCl, KCl, BaCl₂, AlCl₃.

Chemical kinetics

- 1. Determination of rate of decomposition of hydrogen peroxide.
- 2. Determination of specific reaction rate of the hydrolysis of methyl acetate catalyzed by hydrogen ion at room temperature.
- 3. Comparison of strengths of HCl and H₂SO₄ in the kinetic study of hydrolysis of methyl acetate.
- 4. Comparative kinetics of Hydrolysis of methyl acetate and ethyl acetate in the presence of HCl.

- 1. Svehla, G. Vogel's Qualitative Inorganic Analysis, Pearson Education (2012).
- 2. Mendham, J. Vogel's Quantitative Chemical Analysis, Pearson (2009).
- 3. Khosla, B. D.; Garg, V. C. & Gulati, A: Senior Practical Physical Chemistry, R. Chand & Co.
- 4. Alexander Findlay: Practical Physical Chemistry
- 5. B. P. Levitt: Findlay's Practical Physical Chemistry
- 6. P. S. Sindhu: Practicals in Physical Chemistry, A Modern Approach

IPCH-4.4LAB: PHARMACOLOGY LAB (Credits: 2, 3hrs/week)

- 1. Calculation of IC50 values and Ki values with given data using micro soft excel sheet (practice with at least five data sets)
- 2. Identification of agonist and antagonist using dose response curves (interpretation of dose response curves) (practice with at least 10 curves)
- 3. Determination of disintegration time of various types of tablet formulations of a drug
- 4. Determination of disintegration time of tablets of a drug from various manufacturers or batches (three experiments)
- 5. Drug concentration time profiles of various formulations at acidic and neutral buffers (at least 4 formulations)
- 6. Determination of minimum inhibitory concentration of antibacterial agents
- 7. Drawing of antibacterial agents using chem sketch programme and visualizing in 3D view

- 1. H. Gerhard Vogel: Drug Discovery and Evaluation-Pharmacological Assays, 2nd edition, Springer Verlag, Berlin, Heidelberg.
- 2. A. H. Becket and J. B. Stenlake: Practical Pharmaceutical Chemistry, 4th edition, the Athlone press
- 3. Sara E. Rosenbaum: Basic Pharmacokinetics and Pharmacodynamics: An integrated Text Book and Computer Simulations, Wiley publications

IPCH-4.5LAB: GENETIC ENGINEERING LAB (Credits: 2, 3hrs/week)

- 1. Problems on Restriction Mapping
- 2. Restriction Digestion
- 3. Preparation of competent cells
- 4. Identification of competent cells by Blue-white screening
- 5. Preparation and sterilization of medium for animal cell culture
- 6. Culture and maintenance of cell lines
- 7. Viability tests for cell lines
- 8. Preparation and sterilization of MS Media for plant tissue culture
- 9. Induction of Callus
- 10. Suspension culture of plant cells
- 11. Production of Pharmaceutical products by plant tissue culture

SEMESTER-V

IPCH-5.1T: PHYSICAL CHEMISTRY AND TOPICS OF INDUSTRIAL IMPORTANCE (Units: 5, Hours: 60, Credits: 4)

Unit-I: Thermodynamics

Thermodynamic relations-Gibbs equations, Maxwell relations, temperature dependence of G, Gibbs-Helmholtz equation; Pressure dependence of G, Chemical potential-Gibbs equation for non-equilibrium systems, Material equilibrium, Phase equilibrium, Clapeyron equation and Clausius-Clapeyron equation; Derivation of equilibrium constant from thermodynamic consideration, temperature dependence of equilibrium constant-the Van't Haff equation; Chemical potential of ideal gases, Solutions, Partial molar properties-significance; Relation between solution volume and partial molar volumes, Determination of partial molar volumes-slope and intercept methods, Variation of chemical potential with T and P; Gibbs-Duhem equation-derivation and significance, Ideal solutions and thermodynamic properties of ideal solution, Mixing quantities, Vapour pressure-Raoult's law, Thermodynamic properties of ideally dilute solutions, Vapour pressure-Henry's law, Non-ideal systems; Concept of fugacity, fugacity coefficient, determination of fugacity; Non ideal solution, Activities and activity coefficients, Standard-state conventions for non-ideal solutions, Excess functions and their determination, Determination of activity coefficients from vapour pressure measurements, Activity coefficients of nonvolatile solutes using Gibbs-Duhem equation.

Unit-II: Photochemistry-I

Interaction of radiation with matter, difference between thermal and photochemical processes; Law of Photochemistry, Grothus-Draper law and Stark-Einstein law, Quantum yield and its determination, examples of low and high quantum yields (Photochemical combination of hydrogen-bromine and hydrogen-chlorine). Jablonski diagram depicting various processes occurring in the excited state, qualitative description of fluorescence, phosphorescence, non- radioactive processes (Internal conversion, Intersystem crossing); Photosensitized reactions-energy transfer processes (simple examples); Sensitized fluorescence, Quenching of fluorescence, Stern-Volmer equation; Actinometry-ferrioxalate and uranyl oxalate actinometers

Unit-III: Surface Chemistry & Catalysis

BET theory of multilayer adsorption, derivation of BET equation, its limitations and its applications; Introduction catalysis, characteristics of catalytic reactions, types (homogeneous/heterogeneous/bio-/anchored/PTC), characteristics of catalyst, homogeneous and heterogeneous catalysis with examples, activation energy of catalyzed reactions; enzyme catalysis, characteristics of enzyme catalysis, classification of enzyme catalysis, kinetics of enzyme catalysis (Michaelis-Menten kinetics), factors effecting enzyme catalysis; steps in heterogeneous catalyzed reaction, mechanism of surface-catalyzed reactions, the Langmuir -Hinshelwood and the Eley-Rideal mechanism; Determination of surface area by BET method, Determination of pore size and pore volume distribution by BJH method; Some industrially important heterogeneous catalytic processes: heterogeneous catalytic hydrogenation and oxidation, Fischer-Tropsch synthesis, Water-Gas shift reactions, methanol economy.

Unit-IV: Nanomaterials

Overview of nanostructures and nanomaterials (natural and synthetic), definition and classification of nanodimensional materials/particles, important techniques for synthesis of nanomaterials (physical/chemical/biological, top-down/bottom-up); special focus on synthesis of gold and silver nanomaterials; self assembly/stabilization-Moore's theory; optical, electrical and magnetic properties;

characterization techniques (SEM, TEM, AFM, UV-Vis, XRD, POM); scope of applications of nanoparticles/nanomaterials in catalysis, energy, pharmacy, water treatment, food science, optoelectronics, fuel-cell and environment; Carbon related nanostructures (Fullerenes, Graphene, CNTs) properties & applications

Unit-V: Green Chemistry

Introduction, 12 principles of 'Green Chemistry' with appropriate examples, atom economy and scope, green solvents and choice of solvents-water as a solvent for organic reactions, ionic liquids, supercritical fluids, PEG, deep eutectic solvents and solventfree reactions with appropriate examples; Catalysis and green chemistry, phase transfer catalysis in green chemistry

Examples of Green Synthesis/ Reactions and some real world cases:

- i) Green Synthesis of the adipic acid, poly lactic acid and biodiesel
- ii) Microwave assisted reactions in water: Hofmann Elimination
- iii) Microwave assisted reactions in organic synthesis: Diels-Alder reaction
- iv) Ultrasound assisted reactions: Sonochemical Simmons-Smith Reaction (Ultrasonic alternative to Iodine)

- 1. Advanced Physical Chemistry-Gurdeep Raj
- 2. Principles of Physical Chemistry-Puri, Sharma and Pathania
- 3. Physical Chemistry-Walter Moore
- 4. Physical Chemistry-D. A. Mc Quarrie and J.D. Simon
- 5. A text book of Physical Chemistry-Glasstone and Van Nostrand
- 6. A. Zangwill, Physics at Surfaces, Cambridge Univ. Press, 1988.
- 7. Catalytic Chemistry, Wiley, 1992-B. Gates
- 8. Physical Chemistry of Surfaces, Wiley, 1997-A. W. Adamson, A. P. Gast
- 9. Principles and Practice of Heterogeneous Catalysis, 1997- J. M. Thomas and W.J. Thomas
- 10. Surface Science: Foundations of Catalysis and Nanoscience, Wiley, 2002- K. W. Kolasinski
- 11. Heterogeneous Catalysis, New Age, 2008-D.K. Chakrabarty and B. Viswanathan
- 12. Introduction to Surface Chemistry and Catalysis, Wiley, 2010-G. A. Somorjai and Y. Li
- 13. Physical chemistry of surfaces, 1990-Arthur W. Adamson
- 14. Chemical kinetics and catalysis Wiley-Interscience, 2001-R. I. Masel
- 15. An introduction to chemisorption and catalysis by metals, 1985-R. P. H. Gasser
- 16. Introduction to Nanotechnology John Wiley & Sons- Poole, C. P. & Owens, F. J.
- 17. Fundamentals and Applications of Nanomaterials, Artech House-Z. Guo, L. Tan
- 18. Nano: the essentials, Tata McGraw Hill-T. Pradeep
- 19. Nanostructured Materials and Nanotechnology, edited by Hari Singh Nalwa, Academic Press
- 20. Introduction to Nanotechnology-Charles P. Poole Jr, F. J. Owens
- 21. New Trends in Green Chemistry-Ahluwalia, V. K. & Kidwai, M. R.
- 24. Green Chemistry-Theory and Practical, Oxford University Press Anastas, P.T. & Warner, J. K.
- 25. Green Chemistry Experiments:
- 26. A monograph I.K. International Publishing House Pvt Ltd. New Delhi-Sharma, R. K.; Sidhwani, I. T. & Chaudhari, M. K
- 27. An Introduction to Green Chemistry, Vishal Publishing-V. Kumar

IPCH-5.2T: COORDINATION AND SUPRAMOLECULAR CHEMISTRY (Units: 5, Hours: 60, Credits: 4)

Unit-I: Metal-Ligand Bonding Theories and Coordination Equilibria

Theories of metal bonding-VBT, CFT and their limitations (review), experimental evidence for metalligand bond covalency, molecular orbital (MO) theory of selected octahedral and tetrahedral complexes, sigma (σ)- and pi(π)-bonding in complexes, Nephelauxetic effect, Solvation of metal ions, formation of binary metal complexes and their stability, step-wise and overall stability constants relation, factors influencing the stability constants: (i) metal ion effects (charge, size and Irving - William's order) (ii) Ligand effects (basicity, chelate, macro cyclic and cryptate effects), Jahn Teller effect on stability constants of metal complexes, symbiosis (chemical), HSAB concept, Methods used for the determination of stability constants; pH metric and spectrophotometric methods. Ternary metal complexes formation, step wise and simultaneous equilibria with appropriate examples

Unit-II: Reaction Mechanisms of Transition Metal Complexes

Concept of labile and inert complexes in terms of VBT and CFT, types of ligand substitution reactions in octahedral (SN^1 dissociative & SN^2 associative), acid and base hydrolysis reactions of octahedral complexes, factors influencing acid hydrolysis, base hydrolysis and conjugate base (SN^1CB) mechanism, evidence in favour of S_N1CB mechanism, annation reactions, Ligand substitution reactions of square planar metal complexes, trans effect-theories and application; Electron transfer reactions: classification, inner and outer-sphere electron transfer reactions mechanism and evidences for one electron transfer, Marcus-Hush Theory, some examples of two electron transfer reactions.

Unit-III: Electronic Spectra and Magnetic Properties of Transition Metal Complexes

Electronic Spectra-UV-Vis, colors, charge transfer and d-d transitions, intensities and origin of spectra, metal centered electronic spectra of transition metal complexes: microstates, terms of p² and d² configurations, L-S (Russel-Saunders) coupling, spin-orbital coupling parameters, term symbols and splitting of terms in free atoms, hole formalism, energy ordering of terms (Hund's rules), selection rules for electronic transitions, Racah parameters-Orgel diagrams; Types of magnetic behavior (diapara, ferro, ferri and anti-ferro), temperature effect on magnetism, magnetic susceptibility determination by Guoy's method, spin-orbit coupling, quenching of orbital angular momentum on A, E and T ground terms, general applications of magnetic metal compounds in materials and pharmaceutical chemistry

Unit-IV: Molecular Clusters

Main-group clusters: General synthesis, geometric and electronic structure, three, four and higher connect clusters, the *closo-*, *nido-*, *arachno-*borane structural paradigm, Wade-Mingos electron counting rules (polyhedral skeletal electron pair theory)

Transition-metal clusters: General synthesis, factors affecting the formation of metal-metal bond, structure, low nuclearity metal-carbonyl clusters, high nuclearity metal-carbonyl clusters (Fe, Ru, Os Co, Rh, Ir), isolobal analogy, compounds with M-M multiple bonds structure and bonding in $[Re_2Cl_8]^2$, Application of molecular clusters in catalysis, materials, and biology.

Unit-V: Supramolecular Chemistry

Introduction, synonymous terminology in supramolecular chemistry, types of guests (cationic, anionic neutral), types of non-covalent interactions (hydrogen bonding, electrostatic, ring π - π and metal- π interactions, Van der Waals, hydrophobic/solvophobic forces and closed shell interactions); Types of

hosts, stability of host-guest complex/binding constants; Cation binding, binding between metal cation and macrocycles, factors affecting the hole size macrocyclic ligand; Anion binding, properties of anions, design principle, macrocycles with secondary binding sites; Neutral species binding, hydrogen bond receptors, complementary hydrogen bonding receptors, secondary interactions, supplementing hydrogen bonding with other interactions, dendrimers synthesis and applications; Applications in pharmacy, phase transfer reagents, molecular sensors, switches and molecular machinery, catalysis and nanotechnology.

- 1. Basic Inorganic Chemistry, Wiley publishers-Cotton, F. A & Wilkinson, G.
- 2. Inorganic Chemistry Principles of Structure and Reactivity, 4th Edn., Pearson Education India, 2006-J. E. Huheey, E. A. Keiter, R. A. Keiter
- 3. Mechanisms of Inorganic Reaction, John Wiley & Sons-F. Basolo, R. G. Pearson
- 4. Physical Methods in Chemistry, Saunders College-R. S. Drago,
- 5. Ligand Field Theory and its Applications, Wiley, India-B. N. Figgis, M. A. Hitchman
- 6. Selected Topics in Inorganic Chemistry-R D Madan, G D Tuli & Wahid U Malik
- 7. Concise Inorganic Chemistry, 4th Edn, Wiley-India-J. D. Lee,
- 8. Inorganic Chemistry, Oxford University Press-Shriver, D. F. & Atkins, P. W
- 9. Inorganic Electronic Spectroscopy, 2nd Edn, Elsevier publishers-A. B. P. Lever
- 10. The Chemistry of Metal Cluster Complexes-D. F. Shriver, H. D. Kaerz and R. D. Adams
- 11. Supramolecular Chemistry-Concepts and Perspectives (Wiley-VCH, 1995)-J. M. Lehn
- 12. Supramolecular Chemistry (Oxford University Press, 1999)-P. D. Beer, P. A. Gale, D. K. Smith
- 13. Supramolecular Chemistry (Wiley, 2000)-J. W. Steed and J. L. Atwood

IPCH-5.3T: PRINCIPLES OF DRUG DISCOVERY AND DEVELOPMENT (Units: 5, Hours: 60, Credits: 4)

Unit-1: Drug Discovery-An Overview

Over view on drug discovery and drug development scenario; Statistics of drugs available; Overview on top selling drugs; neglected diseases; Sources of leads for drug development; Over view on drugs (with examples) obtained from ethnopharmaceutical sources, Plant sources, Marine sources, Microorganisms and Animal sources; Compound collections and data bases, merits and demerits of few natural leads quinine and curcumin

Unit-2: Pharmacokinetics and Drug Discovery

Introduction to Pharmacokinetics, PK Parameters (Volume of Distribution, Area Under the Curve, Clearance, Half-life, Bioavailability), General classification of pharmacokinetic properties, Drug regimens, Drug concentration analysis and its therapeutic significance, The importance of pharmacokinetics in drug discovery, Pharmacokinetic models, Intravascular administration and distribution, Extravascular administration, dissolution and absorption, Single oral dose, The calculation of t_{max} and C_{max}, Repeated oral doses, use of pharmacokinetics in drug design, Effects of Plasma Protein Binding on PK Parameters, Tissue Uptake, Drug distribution and 'survival', Drug design for pharmacokinetic problems (Variation of substituents, Stereoelectronic modifications etc)

Unit-3: Pharmacodynamics and Drug Discovery

Chemical stability, Metabolic stability and metabolic reactions; stereochemical, biological, and environmental factors effecting metabolism; species and metabolism; enzymes and metabolism; secondary implications of metabolism (Inactive metabolites, toxic metabolites, metabolites with similar activity, metabolites with different activity); sites of action; Hydrophilic/hydrophobic balance; Drug dose levels; Metabolic blockers; Removal of susceptible metabolic groups; 'Sentry' drugs—synergism; 'Search and destroy' drugs; Self-destruct drugs; kinetics of metabolites; metabolism and drug design (Delivery systems).

Unit-4: Drug-like Properties

Leads and analogues, Bioavailability, Solubility, Structure and Stability, Drug-like Properties (Lipinski Rules, Veber Rules), Application of rules for compound assessment, examples for drug properties and discovery inefficiencies, Property Profiling in Discovery, general chemical properties of functional groups, Drug-like Property Optimization in Discovery through prodrugs and bioisosters.

Unit-5: Structural Modification in Drug Discovery

Binding role of hydroxyl, amino groups, aromatic rings, double bonds; Structure-activity relationships of synthetic analogues with variation of substituents, extension of the structure, chain extensions/contractions, degree of unsaturation, ring expansions/contractions, ring variations, simplification of the structure, changing size and shape, rigidification of the structure; introduction of amino group, halogens, hydroxyl, carboxylic groups, sulphonic acid, thiols, sulphides, elements of luck and inspiration, case study of oxaminoquine, SAR of sulfonamides, local anesthetics,

Reference Books

1. Essentials of pharmaceutical chemistry, Donald Cairns, Pharmaceutical Press, ISBN 978-0 85369-745-9

Syllabus for 5yrs Integrated M.Sc Chemistry (Pharmaceutical Chemistry), Effective from AY 2015-16 Department of Pharmaceutical Chemistry, Telangana University, Dichpally, Nizamabad-503322

- 2. Drug like properties: concepts, structure design and methods, from ADME to toxicity optimization, by Edward H. Kerns and Li Di, Elsevier publications, ISBN: 978-0-1236-9520-8
- 3. An introduction to medicinal chemistry, Graham L. Patrick, Oxford University Press
- 4. Medicinal Chemistry, 2nd edition, Gareth Thomas, John Wiley and sons publishers, ISBN 978-0-470-02597-0 (HB), 978-0-470-02598-7 (PB)
- 5. The practice of medicinal chemistry, Camille Georges Wermuth, Elsevier Publications, ISBN 0-12-744481-5
- 6. Foye's principles of medicinal chemistry, Thomos L. Lemke, David A. Williams, Lippincott Williams and Wilkin publishers,
- 7. Transport processes in pharmaceutical systems, Gordon L. Amidon, Ping I. Lee, Elizabeth M. Topp, Marcel Dekker Inc, ISBN: 0-8247-6610-5
- 8. Goodman and Gilman's Manual of pharmacology and therapeutics, McGraw Hill publications
- 9. Basic principles of drug discovery and development, Benzamin E. Blass, Elsevier publications, ISBN: 978-0-12-411508-8

IPCH-5.4T: MOLECULAR TARGETS AND SIGNAL TRANSDUCTION (Units: 5, Hours: 60, Credits: 4)

Brief introduction and role of following targets in pathophysiology and treatment of various diseases to enable student to understand drug action and to facilitate him/ her to think about strategies of new drug discovery

Unit-1: Receptors as Drug Targets

Fundamentals of receptor action; *GPCRs*: Acetyl choline receptors (Muscarinic receptors), Adenosine receptors, Adrenoceptors, Purinergic receptors, dopamine receptors, angiotensin receptors; *Direct ligand gated ion channel receptors*: GABA_A receptors, Acetyl choline receptors (Nicotinic receptors), Glutamate receptors; *Cytokine receptors*: TNF-\alpha receptors, Interleukin receptors; *Receptors associated with tyrosine kinase*: Insulin receptors; *Nuclear receptors* (steroid hormone receptors): progesterone receptors, Mineralocorticoid receptors; *other nuclear receptors*: Peroxisome proliferator-activated receptor (PPAR)

Unit-2: Enzymes as Drug Targets

Fundamentals of enzyme action; *Oxidoreductases:* MAOs, COXs, LOXs, Aromatase, Dihydro folate reductase (DHFR), Xanthine Oxidase; *Transferases:* Protein Kinase-C, COMT, Reverse transcriptase, RNA Polymerase, DNA polymerase, Tyrosine kinases; *Hydrolases (proteases):* Aspartyl proteases; *Hydrolases (metalloproteases):* ACE, Human carboxy peptidase; *Other hydrolases:* Esterases (AChE, PDE, HDAC); *Lyases:* DOPA decarboxylase, carbonic anhydrase; Isomerases, DNA gyrase, topoisomerases; *Ligases (Synthases):* Thymidylate synthase

Unit-3: Ion Channels as Drug Targets:

Introduction; Voltage-gated Ca²⁺ channels (L-Type channels, T-Type channels); K⁺ channels (Epithelial K⁺ Channels, Voltage gated K⁺ Channels); Na⁺ channels (Epithelial Na⁺channels (ENaC), Voltage-gated Na⁺channels); Direct ligand gated ion channels; Ryanodine-inositol 1,4,5-triphosphate receptor Ca²⁺ channel (RIR-CaC) family: Rynodyne receptors, Cl⁻ channels, Acid sensing (Proton gated) Ion channels, Cyclic nucleotide gated (CNG) and hyperpolarization activated cyclic nucleotide gated (HCN) Channels, Transient receptor potential channels (Transient receptor potential Ca2+channel (TRP-CC) family)

Unit-4: Membrane Transporters as Drug Targets, Various Physicochemical Mechanisms

Membrane transporters as drug targets: Fundamentals, effects of transporters, definition of terms: Uniporters, symporters, antiporters; Efflux transporters (MDR, ABC), Uptake transporters, Biogenic amine transporters, Excitatory amino acid transporters, GABA transporters, Glycine transporters, Na⁺/H⁺ antiporters, Proton pump, Cation-chloride co-transporter (CCC) family, Na⁺/K⁺ ATPase; drug action by various physicochemical mechanisms

Unit-5: Nucleic Acids, Ribosomes, Aquaporins as Drug Targets, Targets of Monoclonal Antibodies, Multi targeting Action of Drugs

Nucleic acids: DNA and RNA, Spindle as drug targets; *Ribosome:* 30S, 50S units as drug targets; *Targets of monoclonal antibodies:* TNF, Immunoglobulins, VEGF, EGFR; Aquaporins as drug targets; *Multi targeting action of drugs:* Introduction, Multi target pharmacology in Alzheimer's disease and cancer, basic considerations, its possibilities and limitations

- 1. The handbook of receptor classification and signal transduction, Published by Sigma-Aldrich
- 2. Drug like properties: concepts, structure design and methods, from ADME to toxicity optimization, by Edward H. Kerns and Li Di, Elsevier publications, ISBN: 978-0-1236-9520-8
- 3. An introduction to medicinal chemistry, Graham L. Patrick, Oxford University Press
- 4. Drugs, their targets and the nature and number of drug targets, Peter Imming, Christian Sinning and Achim Meyer, Nature Reviews Drug Discovery, 5, 821-834, 2006, doi:10.1038/nrd2132
- 5. Drugs and their molecular targets: An updated overview, Yves Landry, Jean-Pierre Gies, Fundamental & Clinical Pharmacology 22 (2008) 1–18; doi:10.1111/j.1472-8206.2007.00548.x
- 6. Basic principles of drug discovery and development, Benzamin E. Blass, Elsevier publications, ISBN: 978-0-12-411508-8
- 7. www.animalsimulator.com
- 8. https://www.rcsb.org/

IPCH-5.5T: PRINCIPLES OF STEREOCHEMISTRY

(Units: 5, Hours: 60, Credits: 4)

Unit-I: Introduction

Isomerism definition, isomerism classification-constitutional isomerism and stereo isomerism; stereoisomerism-conformational isomerism and configurational isomerism; configurational isomerism-geometrical isomerism and optical isomerism

Constitutional isomerism: Definition and classification.

Molecular representations, symmetry and chirality: Wedge, Fischer, Sawhorse and Newman representations and their inter conversion; symmetry operations, symmetry elements $(C_n \& S_n)$ and criteria for chirality.

Conformational isomerism: Definition, conformations, stability and energy profile diagrams of ethane, propane and n-butane; conformations, stability and energy profile diagram of cyclobutane, cyclopentane and cyclohexane.

Unit-II: Conformational Analysis (Acyclic Systems)

Concept of dynamic stereochemistry, conformational enantiomers and conformational diastereomers; study of conformations of 1,2-disubstitued ethane derivatives like 1,2-dichloro ethane, ethylene chlorohydrin, ethylene glycol, butane-2,3-diol and (2-(N,N-dimethylamino)-1,2-diphenyl ethanol; study of conformations of unsaturated acyclic compounds like propylene, 1-butene, acetaldehyde, propionaldehyde; Klyne-Prelog terminology for torsion angles; quantitative analysis of conformation-reactivity relationship by the Winstein-Holness equation and the Curtin-Hammett principle; introduction to use of physical and spectral methods in conformational analysis.

Unit-III: Conformational Analysis (Cyclic Systems)

Study of conformations of mono, di and poly substituted cyclohexanes, cyclohexene, cyclohexanone (2-alkyl & 3-alkyl ketone effect) 2-halocyclohexanones, cycloheptane, cyclooctane; conformational analysis of fused bicyclic systems like bicyclo[3,3,0]octane, bicyclo[4,3,0]nonane (hydrindanes) and decalins; conformational analysis of heterocycles like piperidine, N-methylpiperidine, tropane, tropine and pseudotropine; reactivity of cyclohexane with axial and equatorial substituents; stereochemistry of addition to the carbonyl group of a rigid cyclohexanone ring

Unit-IV: Configurational Isomerism

Geometrical isomerism: Cis/Trans isomerism, E&Z nomenclature; spectral and chemical methods of configuration determination of E&Z isomers, determination of configuration of aldoximes and ketoximes

Optical isomerism: Definition, enantiomers, diastereomers, relationship between enantiomers and diastereomers; examples of asymmetric molecules (Glyceraldehyde, Lactic acid, Alanine) and disymmetric molecules (trans-1,2-dichlorocyclopropane); molecules with constitutionally symmetrical chiral carbons (Tartaric acid); molecules with constitutionally unsymmetrical chiral carbons (2,3-dibromopentane); R&S nomenclature (CIP), specific optical rotation (SOR), measurement of optical rotation, factors affecting the optical rotation

Unit-V: Techniques

Racemisation and resolution techniques: Racemisation methods (by mixing, synthesis and thermal) and resolution by direct crystallization, diastereoisomer salt formation and chiral chromatography

Determination of absolute configuration: Determination of absolute configuration by chemical correlation methods

Axial chirality, planar chirality and helicity: Stereochemistry of allenes, spiranes, chiral biphenyls (Atropisomerism), ansa compounds, trans-cyclooctane and helically chiral compounds

- 1. Stereochemistry and mechanism through solved problems P. S. Kalsi
- 2. Stereochemistry of organic compounds D. Nasipuri
- 3. Stereochemistry of carbon compounds Ernest L Eliel
- 4. Stereochemistry conformation and mechanism P. S. Kalsi (9th edition)
- 5. Advanced organic chemistry Jerry March
- 6. Advanced organic chemistry Francis A Carey & Richard Sundberg
- 7. Organic chemistry Clayden, Greeves, Warren & Wothers

IPCH-5.3LAB: PRINCIPLES OF DRUG DISCOVERY AND DEVELOPMENT LAB (Credits: 2, 3hrs/week)

- 1. Molecular representations of few natural products
- 2. Determination of partition coefficient of various drugs
- 3. Prediction of physicochemical properties of few compound libraries
- 4. Determination of pharmacokinetic parameters of paracetamol using *in vitro* dissolution experiment
- 5. Investigations on stability of drugs in gastric environment and comparison with its prodrugs
- 6. Prediction of drug likeliness of few compound libraries
- 7. Prediction of metabolic stability of few compound libraries
- 8. In vitro absorption studies of various formulations of drugs
- 9. In vitro evaluation of compounds for antioxidant activity
- 10. Structure and activities of various drugs

IPCH-5.4LAB: MOLECULAR TARGETS AND SIGNAL TRANSDUCTION LAB (Credits: 2, 3hrs/week)

- 1. Potential drug databases
- 2. Potential protein databases
- 3. Various protein visualizing softwares
- 4. Visualizing protein structures in protein databank
- 5. Visualizing protein ligand interactions with co-crystallized structures
- 6. Evaluation of drugs using various enzyme assays (in vitro)
- 7. Simulations of animal experiments demonstrating role of various targets in activity of drugs

IPCH-5.5LAB: ORGANIC SYNTHESIS LAB (Credits: 2, 3hrs/week)

Synthesize the following compounds, purify and recrystallize as per the procedures. Analyze the synthesized compounds by TLC; melting points/boiling points by comparing with the standard samples. Calculate the moles, equivalents and yields.

Nitro benzene, *p*-Bromo acetanilide, *m*-Nitro aniline, Aspirin, Acetanilide, Benzylideneaniline, 2-Naphthyl methyl ether (Neroline), Nitrobenzoic acid and *n*-Butyl acetate

- 1. Vogel, A. I., Tatchell, A. R., Furnis, B. S., Hannaford, A. J. & Smith, P. W. G: Textbook of Practical Organic Chemistry, Prentice-Hall, 5th edition (1996).
- 2. Mann, F. G. & Saunders, B. C: Practical Organic Chemistry Orient-Longman (1960).
- 3. Ahluwalia, V.K. & Aggarwal, R: Comprehensive Practical Organic Chemistry.

SEMESTER-VI

IPCH-6.1T: REAGENTS AND REACTION MECHANISM (Units: 5, Hours: 60, Credits: 4)

Unit-I: Protecting Groups

Role of protecting groups in organic synthesis, and the protection and de-protection of the following functional groups with examples

- a) Protection of alcohols as ethers (MOM, PMB, THP, trityl), silyl ethers and esters
- b) Protection of 1,2-diols as cyclic acetal/ketal and cyclic carbonates
- c) Protection of carbonyls as acetal, ketal (as well as cyclic ethers) and thioacetal (Umpolung)
- d) Protection of amines as amides (acetylation, benzoylation), carbamates (Cbz, BOC, Fmoc)
- e) Protection of carboxylic acids as ester and ortho ester

Unit-II: Oxidizing Reagents

- (a) Oxidation of alcohols: Cr(VI) oxidants (Jones reagent, PCC, PDC), DMP, TEMPO, Swern oxidation, silver carbonate, MnO₂
- b) Dihydroxylation of alkenes: Prevost and Woodward
- c) Oxidative cleavage of diols: Periodic acid and lead tetracetate
- d) Oxidation of allylic and benzylic C-H bonds: DDQ and SeO₂

Unit-III: Reducing Reagents

- a) Catalytic hydrogenation: homogenous and heterogeneous catalytic reduction
- b) Nucleophilic metal hydrides: LiAlH₄, NaBH₄
- c) Electrophilic metal hydrides: BH3 and AlH3 and DIBAL
- d) Non-metallic reductions: diimide reduction.
- e) Dissolving metal reductions: Birch reduction
- f) Hydrogenolysis: use of tri-n-butyl tin hydride

Unit-IV: Reaction Mechanism-I

Elimination reactions: $\Box \Box \Box \Box \Box and \Box \Box$ -eliminations; E1, E2 and E1cb mechanisms; orientation and stereochemistry of elimination reactions, dehydration, pyrolytic *syn* elimination, elimination Vs substitution

Electrophilic addition to C=C: (a) *anti* addition with examples (b) syn addition with examples (c) addition to conjugated dienes (1,2-addition Vs 1,4-addition)

Nucleophilic addition: to α,β -unsaturated nitriles and α,β -unsaturated carbonyls

Nucleophilic aromatic substitution: SN1(Ar), SN2(Ar), and benzyne mechanisms, benzyne generation and evidence for the structure of benzyne, Von Richter rearrangement, Definition and reactions of ambient nucleophiles

Unit-V: Reaction Mechanism-II

Neighboring Group Participation (NGP): Criteria for determining the participation of neighboring group; enhanced reaction rates and retention of configuration; isotopic labeling and cyclic intermediates; neighbor group participation involving halogens, oxygen, sulphur, nitrogen, aryl, cycloalkyl groups, σ and π - bonds; introduction to non-classical carbocations

Investigation of reaction mechanism: Nature of the products, kinetic data, transition states, study of intermediates, use of isotopes, chemical trapping and crossover experiments; use of IR and NMR in the investigation of reaction mechanism

- 1. Mechanism in organic chemistry-Peter Sykes
- 2. Organic reaction mechanisms-Raj K Bansal
- 3. Name reactions: Collection of detailed mechanisms & synthetic applications-Jie Jack Li
- 4. Reaction mechanisms in Organic Chemistry-Mukul C Ray
- 5. Organic Reaction and Molecular Rearrangements with Mechanism-S Kalaivani
- 6. Mechanisms in organic reactions-Richard A Jackson
- 7. The investigation of organic reactions and their mechanisms Howard Maskill
- 8. Advanced organic chemistry reaction mechanisms-Reinhard Bruckner
- 9. Advanced organic chemistry-Jerry March
- 10. Advanced organic chemistry- Francis A Carey & Richard Sundberg
- 11. Mechanism and structure in organic chemistry-S Mukerjee
- 12. Organic chemistry-Clayden, Greeves, Warren & Wothers
- 13. Protective groups in organic synthesis-Peter G M Wuts& Theodora W Greene
- 14. Handbook of reagents for organic synthesis: Activating agents and protecting groups-A J Pearson & William R Roush
- 15. Handbook of reagents for organic synthesis: Oxidizing and reducing agents- Steven D Burke & Rick L Danheiser
- 16. Handbook of reagents for organic synthesis: Acidic and Basic Reagents-Hans J Reich & James H Rigby
- 17. Handbook of reagents for organic synthesis: Activating agents and protecting groups-Anthony J Pearson & William R Roush
- 18. Handbook of reagents for organic synthesis (Vol. IV)-Reich and Rigby
- 19. Reagents in organic synthesis-B P Mundy and others
- 20. Name reactions and reagents in organic synthesis-Bradford P Mundy, Michael G Ellerd & Frank Favaloro

IPCH-6.2T: CHEMISTRY OF MAIN GROUP ELEMENTS

(Units: 5, Hours: 60, Credits: 4)

Unit-I: Compounds of Hydrogen and S-block Elements (Alkali and alkaline earth metals)

Review of periodicity and diagonal relationship in main group, metallic and non-metallic nature, polyanions/cations of main group; chemistry of hydrogen: binary compounds of hydrogen, classification of hydrides (ionic, covalent, and metallic/non-metallic hydrides); chemistry of S-block elements metals: extraction of S-block metals with crown ethers and cryptands, solvation and complexation tendencies of S-block metals including their function in biosystems, reactions of S-block metals with non-metals and water, ion-pumps and ion transport, application of S-block metals and their compounds in agriculture, materials and pharmaceutical chemistry; characteristics of battery; working of Pb-acid and Li-Battery

Unit-II: Compounds of P-block Elements-I

Inert pair effect and low valent compounds, Allotropy (polymorphism) and catenation of C, S, and P; multiple bonding in heavier main-group elements (Si=Si, Si=Si, P=P, Bi=Bi bonds); new Lewis acids and bases, polymer-supported Lewis acids; inorganic chains, cages, clusters, rings (homo/heterocyclic) and polymers of main group elements; Boranes, Boron oxides, B-N compounds, Carbides, Silanes, Silicates, Silicones, Si-N, P-N, S-N and P-S compounds

Unit-III: Compounds of P-block Elements-II

Chemistry of oxides and oxy-acids of N_2 , P, S and Halogens; oxidation states of nitrogen and their inter-conversion; N_2 and S oxides and their redox chemistry and their effect in environment; hypervalent molecules, hypervalent-halogen compounds, inter-halogens, molecular halides, pseudohalides, noble gas compounds

Unit-IV: Selected Topics of Main Group Materials

Glass: glassy state, classification (silicate/non-silicate), manufacture, composition and properties; Ceramics: types of ceramics (important clays), high technology ceramics and their applications; Cements: classification of cement, ingredients and their role, manufacture of cement and the setting process, quick setting cements; Zeolites and clay: hetero-polyacids formed by main group, Hydrotalcites, Hydroxyapatites; Fertilizers: different types of fertilizers, manufacture of the following fertilizers: Urea, ammonium nitrate, calcium ammonium nitrate, ammonium phosphates; polyphosphate, superphosphate, compound and mixed fertilizers, potassium chloride, potassium sulphate; introduction to rocket propellants (solid/liquid/gas)

Unit-V: Coordination, Organoelement/Organometallic Chemistry of Main Group

Organometallic compounds of Li, Mg, Be: classification, synthesis, properties, uses; Aluminum alkyls and use of Aluminum alkyls in polymerization of olefins; organometallic compounds of Si, Sn, Pb, Ga, As, Sb, Bi: structures, synthesis, reactions; basic characterization techniques of main-group and organometallic compounds (NMR, Mass, IR); Organoboranes, Organosilanes,

- 1. General Chemistry, 5th Ed. Macmillan Publishing Co-Petrucci, R. H
- 2. Basic Inorganic Chemistry, Wiley- Cotton, F. A. & Wilkinson, G
- 3. Inorganic Chemistry, Oxford University Press- Shriver, D. F. & Atkins, P. W.
- 4. Inorganic Chemistry, Viva Books Pvt. Ltd- Wulfsberg, G

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- 5. Inorganic & Solid State Chemistry, Cengage Learning India Ltd (2008)- Rodgers, G. E
- 6. Inorganic Chemistry Principles of Structure and Reactivity, 4th Edn., Pearson Education India, 2006-J. E. Huheey, E. A. Keiter, R. A. Keiter
- 7. Mechanisms of Inorganic Reaction, John Wiley & Sons-F. Basolo, R. G. Pearson
- 8. Physical Methods in Chemistry, Saunders College-R. S. Drago,
- 9. Ligand Field Theory and its Applications, Wiley, India-B. N. Figgis, M. A. Hitchman
- 10. Selected Topics in Inorganic Chemistry-R D Madan, G D Tuli & Wahid U Malik
- 11. Concise Inorganic Chemistry, 4th Edn, Wiley-India-J. D. Lee,
- 12. Inorganic Chemistry, Oxford University Press-Shriver, D. F. & Atkins, P. W
- 13. Inorganic Electronic Spectroscopy, 2nd Edn, Elsevier publishers-A. B. P. Lever
- 14. The Chemistry of Metal Cluster Complexes-D. F. Shriver, H. D. Kaerz and R. D. Adams
- 15. Supramolecular Chemistry-Concepts and Perspectives (Wiley-VCH, 1995)-J. M. Lehn
- 16. Supramolecular Chemistry (Oxford University Press, 1999)-P. D. Beer, P. A. Gale, D. K. Smith
- 17. Supramolecular Chemistry (Wiley, 2000)-J. W. Steed and J. L. Atwood

IPCH-6.3T: QUALITY CONTROL OF BULK DRUGS AND FORMULATIONS (Units: 5, Hours: 60, Credits: 4)

Unit-I: Quality Control of Excipients

GMP for raw materials, tests related to excipients such as bulk density, tapped density, particle size distribution, pH, moisture content, viscosity (dynamic), gelling temperature, swelling temperature, loss on drying, residue on ignition, conductivity, congealing range, readily carbonizable substances and readily oxidizable substances, melting point, melting range and preservative challenge test; excipients of interest-disintegrating agents, binders, emulsifiers, viscosity modifiers and preservatives

Unit-II: Quality Control of Dosage Forms and Nutraceuticals

In process quality control tests carried on the tablets, capsules, parenterals, liquid orals; quality control of vitamins (A, B1, B2, B12, C, D, E and K); quality control of food constituents-carbohydrates, proteins, fats with emphasis on the determination of moisture, ash, nitrogen and physical constants; analytical methods for testing milk

Unit-III: Product Performance and Stability

Study of chemical properties of drug-hydrolysis, oxidation, reduction, racemization, polymerization and their influence on formulation and stability of the products; bioavailability, bioequivalence, degradation kinetics; stability testing of drugs and pharmaceuticals; accelerated stability studies, interpretation of kinetic data (API & Formulations), shelf-life assignment

Unit-IV: Impurity Profiling of Pharmaceuticals

Sources of impurities, their effect on drug stability and therapeutic actions, acceptance criteria for impurities in drug substances, determination of impurities in bulk drugs and formulations, isolation, characterization and analytical methods with case studies

Unit-V: Drug Regulatory Requirements

National drug policy; Drugs and Cosmetics Act and its amendments, overview of schedules, study of schedule M and Y, ICH guidelines, CDSCO, USFDA, FDA guidelines on IND, NDA and ANDA approvals, and SUPAC changes and understanding on 505 (b) (2) applications

- 1. Pharmaceutical Chemistry-Beckett and Stanlake
- 2. Quantitative analysis of drugs in pharmaceutical formulations-P. D. Sethi
- 3. Pharmaceutical analysis-Higuchi, Bechmman and Hassan
- 4. Theory and practice of industrial pharmacy-Lieberman and Lachman
- 5. Handbook of isolation and characterization of impurities in pharmaceuticals-S. Ahuja, K. M. Alsante, Academic Press, California, 2003
- 6. Remington's Pharmaceutical Sciences-Alfonso and Gennaro
- 7. The chemical analysis of foods-David Pearson, 7th Ed, Churchill Livingstone, Edinburgh, 1976
- 8. Introduction to the chemical analysis of foods-S. Nielsen, Jones & Bartlett Publishers, Boston, 1974
- 9. Indian Pharmacopoeia
- 10. Original laws published by Govt. of India
- 11. Law and Drugs, Law Publications-S. N. Katju

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- 12. Laws of drugs in India-Hussain
- 13. New drug approval process-Guarino, 5th Edn
- 14. Commercial manual on Drugs and Cosmetics 2004, 2nd edition
- 15. Drugs and Cosmetics Act-Vijay Malik
- 16. Good manufacturing practices for pharmaceuticals-S. H. Wiling, Vol. 78, Marcel Decker
- 17. fda.org, wipo.int, patentlawlinks.com, hc-sc.gc.ca, ich.org, cder.org
- 18. Drug regulatory affairs-C. V. S. Subramanyam
- 19. Current good manufacturing practices for pharmaceuticals-Manohar A. Potdar

IPCH-6.4T: SPECTROSCOPY TECHNIQUES (Units: 5, Hours: 60, Credits: 4)

Discuss briefly about light and its effect on molecules when applied with different wave lengths

Unit-I: UV Spectroscopy

Introduction, instrumentation and theory of UV spectroscopy; types of electronic transitions in molecules and formation of absorption bands; chromophore, auxochrome, absorption and intensity shifts; Woodward-Fieser rules for calculating absorption maxima in conjugated dienes, trienes and polyenes, unsaturated carbonyl compounds, benzene and its derivatives, polynuclear aromatic hydrocarbons and diketones; applications of UV spectroscopy

Unit-II: Infrared & Raman Spectroscopy

Introduction and instrumentation of IR spectroscopy; molecular vibrations, factors influencing the vibrational frequencies (electronic and vibrational), calculation of vibrational frequency using Hook's law, fundamental bands, overtones and hot bands, Fermi resonance, finger print region; applications of IR spectroscopy in identification of functional groups, study reaction mechanism, stereochemical effects on absorption pattern of the carbonyl group, cis/trans isomerism and hydrogen bonding; Raman effect, stokes and anti-stokes, comparison of IR and Raman spectra, complementary nature of IR and Raman spectra

Unit-III: ¹HNMR Spectroscopy

Introduction, principle and instrumentation of NMR, continuous wave (CW) and FT-NMR; equivalent and non equivalent protons, enantiotopic and diastereotopic protons; chemical shifts and factors affecting the chemical shifts, electro negativity-shielding and deshielding, anisotropic effect, influence of restricted rotation (in DMF and cyclohexane); solvents used in NMR; signal integration, Spin-Spin coupling: vicinal, geminal and long range coupling, multiplicity, Pascal's triangle, coupling constants and factors affecting coupling constants; protons on hetero atoms-exchangeable; ¹H NMR spectra of ethanol, ethyl acetate, 2-butanone, paracetamol, aspirin, ethyl benzoate, benzyl acetate, 2-chloro propionic acid, identification of cis/trans isomers

Unit-IV: Mass Spectroscopy

Introduction, principle and instrumentation of mass spectrometer (EI); 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 ions; hard ionization techniques: Electron Impact (EI), Chemical Ionization (CI); soft ionization techniques: Fast Atom Bombardment (FAB), Electro Spray Ionization (ESI) and Matrix Assisted Laser Desorption Ionization (MALDI); mass analysers: quadrupole mass analyser, Time of Flight (TOF) mass analyser, Trapped ion mass analyser; Principle of Electron Spray Ionization (ESI) mass spectrometry, Matrix Assisted Laser Desorption Ionization (MALDI) mass spectrometry, GC-MS and LC-MS

Unit-V: Electron Spin (Paramagnetic) Resonance (ESR/EPR)

Introduction, principle and instrumentation of ESR, hyperfine coupling, zero field splitting, factors affecting g values, Kramer's degeneracy, application of ESR spectra to study free radicals like hydrogen, methyl, 1,4-semibenzoquinone, naphthalene, transition metal complexes (Copper(II), Vanadyl(II) and Manganese(II)) and biological systems

- 1. Spectroscopic methods in organic chemistry-D.H. Williams and I. Fleming
- 2. NMR-From Spectra to Structures (2007)-Terence N Mitchell & Burkhard Costisella
- 3. Fundamentals of molecular Spectroscopy-C N Banwell
- 4. Introduction to molecular spectroscopy-G M Barrow
- 5. Organic spectroscopy-William Kemp
- 6. Spectroscopy of organic compounds-P S Kalsi
- 7. Elementary organic spectroscopy-Y R Sharma
- 8. Spectrometric identification of organic compounds-R M Silverstein, G C Bassler& T C Morrill
- 9. Handbook of spectroscopy-G Gauglitz& T Vo-Dinh
- 10. NMR spectroscopy explained-Neil E Jacobsen
- 11. NMR spectroscopy-Joseph B Lambert & Eugene P Mazzolla
- 12. High resolution NMR techniques in organic chemistry-Timothy D W Claridge
- 13. IR and Raman spectroscopy-Siegfried Wartewig

IPCH-6.5T: QUANTUM CHEMISTRY, ELECTROCHEMISTRY AND POLYMERS (Units: 5, Hours: 60, Credits: 4)

Unit-I: Quantum Chemistry-I

Black body radiation-Planck's concept of quantization, Planck's equation, average energy of an oscillator (derivation not required); wave particles duality and uncertainty principle-significance of these for microscopic entities; emergence of quantum mechanics, wave mechanics-derivation of Schrodinger wave equation; physical interpretation of wave function; well behaved functions; normalized and orthogonal functions.

Operators-operator algebra; commutation of operators, linear operators; complex functions; Hermitian operators; operators V and V^2 ; Eigen functions and Eigen values; degeneracy; linear combination of Eigen functions of an operator; postulates of quantum mechanics; observables and operators; measurability of operators; average values of observables; the time dependent Schrodinger equation; separation of variables and the time independent Schrodinger equation; theorems of quantum mechanics; real nature of the Eigen values of a Hermitian operator and significance; orthogonal nature of the Eigen values of a Hermitian operator and significance of orthogonality; expansion of a function in terms of Eigen values; Eigen functions of commuting operators and significance; simultaneous measurement of properties and the uncertainty principle

Unit-II: Solid State Chemistry

Magnetic properties of solids: Classification of magnetic materials, magnetic susceptibility, Langerin diamagnetism, Weiss theory of paramagnetism; 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 Tc superconductivity in cuprates; Phase diagram of Y-Ba-Cu-O system; crystal structure of YBa2Cu3O7-x; preparation of 1-2-3 materials; origin of high Tc superconductivity

Unit-III: Electrochemistry

Electrochemical cells: Chemical and concentration cells (with and without transference); Liquid Junction Potential (LJP), derivation of the expression for LJP-its determination and elimination; applications of EMF measurements, potentiometric titrations; determination of pH from EMF measurements; decomposition potential and its significance; electrode polarization-its causes and elimination; concentration over-potential

Unit-IV: Polymer Chemistry

Classification of polymers, molecular forces and chemical bonding in polymers; polymerization: addition polymerization, free radical addition polymerization, ionic polymerization (both cationic and anionic); polymerization inhibitors, degree of polymerization; chain length in polymers, configuration in polymer chains-stereo regular polymers, co-ordination polymers; Ziegler-Natta catalysis: mechanism; condensation polymerization and its characteristics; molecular weight of polymers-the number average molecular weight and the weight average molecular weight

Unit-V: Kinetics of Polymerization

Mechanism and kinetics of step growth, radical chain growth, ionic chain (both cationic and anionic) and coordination polymerizations; mechanism and kinetics of copolymerization, polymerization techniques (bulk, solution, emulsion and suspension polymerisation); preparation, properties and applications of polymers-Polystyrene, PolyVinylChloride (PVC), Polyethylene, polyacrylonitrile,

polytetrafluro ethylene, Nylon-6,6, terylene; characteristics of an ideal polymer and applications of polymers in pharmaceutical formulations

- 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
- 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. Elementary Quantum Chemistry-F. L. Pilar; McGraw Hill.
- 8. Quantum Chemistry-D. A. McQuarrie; Viva Publications
- 9. Introduction to Solids-Leonid V. Azaroff; Tata McGraw Hill
- 10. Solid state chemistry-D. K. Chakrabarthy; New Age International
- 11. Solid state chemistry and its applications-A. R. West; Plenum
- 12. Polymer Chemistry-An introduction- R. B. Seymour and C. E. Carraher; Marcel Dekker Inc. New York, 1981
- 13. Principals of polymerization-G. Odian; 4th Edn, Wiley, 2004
- 14. Textbook of polymer Sciences-F. W. Billmeyer, 2nd Edn. Wiley Inter sciences, 1971
- 15. Polymer science & technology-P. Ghosh; Tata Mc Graw- Hill Education, 1991
- 16. Kinetics and mechanism of chemical transformations-J. Rajaraman and J. Kuriacose
- 17. Introduction to electrochemistry-S. Glasstone
- 18. Modern electrochemistry-J. O. M. Bockris & A. K. N. Reddy; Plenum

IPCH-6.3LAB: QUALITY CONTROL OF BULK DRUGS AND FORMULATIONS LAB (Credits: 2, 3hrs/week)

- 1. Limit tests for Chlorides, Sulphates, Iron, Lead, Arsenic
- 2. Determination of bulk density, tapped density and true density f APIs
- 3. Determination of flow properties of bulk drugs
- 4. Determination of particle size of bulk drugs
- 5. Determination of pH and pKa of drugs
- 6. Determination of moisture content, ash content, loss on drying, residue on ignition of drugs
- 7. Determination of impurities in bulk drugs and formulations
- 8. Analysis of quality of milk
- 9. Quality control tests for tablets
- 10. Quality control tests for liquid orals
- 11. Quality control tests for parenterals
- 12. Quality control tests for capsules
- 13. Estimation of effect of binders on quality of tablets
- 14. Estimation of solid state stability of bulk drugs
- 15. Assay of vitamins

- 1. Pharmaceutical Chemistry-Beckett and Stanlake
- 2. Quantitative analysis of drugs in pharmaceutical formulations-P. D. Sethi
- 3. Pharmaceutical analysis-Higuchi, Bechmman and Hassan
- 4. Theory and practice of industrial pharmacy-Lieberman and Lachman
- 5. Handbook of isolation and characterization of impurities in pharmaceuticals-S. Ahuja, K. M. Alsante, Academic Press, California, 2003
- 6. Remington's Pharmaceutical Sciences-Alfonso and Gennaro
- 7. The chemical analysis of foods-David Pearson, 7th Ed, Churchill Livingstone, Edinburgh, 1976
- 8. Introduction to the chemical analysis of foods-S. Nielsen, Jones & Bartlett Publishers, Boston,1974
- 9. Good manufacturing practices for pharmaceuticals-S. H. Wiling, Vol. 78, Marcel Decker

IPCH-6.4LAB: SYNTHESIS & SPECTROSCOPY LAB

(Credits: 2, 3hrs/week)

Syntheses of the following compounds:

p-Bromoaniline, 2,4,6-tribromoaniline, 1,3,5-tribromobeznene, Aspirin, Tetrahydrocarbazole, 7-hydroxy-4-methyl coumarin, *m*-dinitrobezene, *m*-nitroaniline, hippuric acid, azalactone, anthracenemaleic anhydride adduct, Pthalimide, 2, 4-dihydroxyacetophenone

Identification of known organic compounds by spectral methods (IR and NMR):

p-Bromoaniline, Toluene, Phenylacetylene, Phenylethylene, n-Butylamine, 1-Bromopropane, Ethyl bromide, Ethyl benzoate, Ethylbenzene, Ethyl acetate, Benzoic acid, Benzaldehyde and 2-Butanone

- 1. Vogel, A. I., Tatchell, A. R., Furnis, B. S., Hannaford, A. J. & Smith, P. W. G: Textbook of Practical Organic Chemistry, Prentice-Hall, 5th edition (1996)
- 2. Mann, F. G. & Saunders, B. C: Practical Organic Chemistry Orient-Longman (1960)
- 3. Ahluwalia, V.K. & Aggarwal, R: Comprehensive Practical Organic Chemistry
- 4. Organic spectroscopy-William Kemp
- 5. Spectrometric identification of organic compounds-R M Silverstein, G C Bassler& T C Morrill

IPCH-6.5LAB: PHYSICAL CHEMISTRY LAB (Credits: 2, 3hrs/week)

Potentiometry

- 1. Titration of strong acid Vs strong base
- 2. Titration of weak acid Vs strong base
- 3. Titration of Fe⁺² Vs Cr₂O₇⁺² (redox titration)
- 4. Potentiometric precipitation titration of Cl Vs Ag⁺
- 5. Determination of solubility product of a sparingly soluble salt like AgCl

p^H Metry

- 1. Calibration of a p^H meter and measurement of P^H of different solutions.
- 2. Preparation of Phosphate buffers.

Solutions

1. Determination of molecular weight of a non-volatile substance by cryoscopic method

Chemical Kinetics

- 1. Peroxydisulphate-I reaction (overall order)
- 2. Oxidation of iodide ion by hydrogen peroxide-iodine clock reaction
- 3. Stoichiometry of peroxydisulphide-iodide reaction
- 4. Peroxydisulphide-iodide reaction: order w.r.t (I) by isolation method

- 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-VII

IPCH-7.1T: SPECTROSCOPIC TECHNIQUES-II

(Units: 5, Hours: 60, Credits: 4)

Unit-I: 1HNMR Spectroscopy-II

First order and non first order spectra: AX, AX2, AX3, A2X3, AMX and AB, ABC, simplification of complex spectra: increased field strength, deuterium exchange and double resonance techniques; discrimination of enantiomers by use of chiral NMR solvents (CSAs), chiral lanthanide shift reagents, Mosher's acid, Nuclear Overhauser enhancement (NOE); Fluxional molecules-bullvalene, [η 5-C5H5M], [η 5-(C5H5)2 Ti η 1-(C5H5)2] and [η 4C8H8Ru(CO)3]; introduction to MRI, solid state NMR: Magic Angle Spinning (MAS) and applications of solid state NMR; applications of NMR in the study of reaction mechanism, keto-enol tautomerism, hydrogen bonding

Unit-II: 13CNMR Spectroscopy

CW and PFT techniques; types of 13CNMR spectra-undecoupled, proton-decoupled and off resonance decoupled (ORD) spectra; 13CNMR chemical shifts, factors affecting the chemical shifts and calculation of chemical shifts of alkanes, alkenes and alkynes; homo nuclear (13C-13C J) and hetero nuclear (13C-1H J and 13C-2H J) couplings; applications of 13CNMR spectroscopy: structure determination, stereochemistry, reaction mechanisms and dynamic processes in organic molecules; 13CNMR spectral editing techniques: principle and applications of APT, INEPT and DEPT methods

Unit-III: 2D NMR Techniques

Principles of 2D NMR; classification of 2D NMR experiments: COrrelation SpectroscopY (COSY) HOMO COSY (1H-1H), TOCSY (TOtal Correlation SpectroscopY, 1H-1H), 2D-INADEQUATE (13C-13C); Hetero COSY (1H-13C/15N-HMQC/HSQC), long range Hetero COSY (1H-13C/15N-HMBC), Homonuclear and Heteronuclear 2D-J-resolved spectroscopy, NOESY and 2D NMR applications

Unit-IV: ORD and CD

Optical Rotatory Dispersion (ORD) and Circular Dichroism (CD) Spectroscopy: optical rotation, circular birefringence, circular dichroism and Cotton effect; plain curves and anomalous curves; empirical and semi empirical rules-the axial haloketone rule, the octant rule, helicity rule, exciton chirality method-exciton coupling between identical chromophores

Unit-V: Mass Spectroscopy-II

Common mass fragmentation pattern of organic compounds-Cleavage of one, two and more bonds; dehydration, dehydrohalogenation, Decarboxylation (eliminations); fragmentation of alkanes, alkenes (allylic cleavage), cycloalkanes, cycloalkenes (retro Diels-Alder fragmentation) cycloalkanols, cycloalkanones and cycloalkyl amines, alkyl substituted aromatic compounds (benzylic cleavage), phenols, aldehydes, ketones, carboxylic acids, esters, amides, amines, alcohols, McLafferty rearrangement, effect; interpretation of the fragmentation pattern of simple organic compounds; EI mass spectra of Limonene, codeine bupivacaine (α -cleavage), chloroquine, propranolol, famotidine and butorphanol

- 1. Spectroscopic methods in organic chemistry-D H Williams and I Fleming
- 2. NMR-From Spectra to Structures (2007)-Terence N Mitchell & Burkhard Costisella
- 3. Fundamentals of molecular Spectroscopy-C N Banwell

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- 4. Introduction to molecular spectroscopy-G M Barrow
- 5. Organic spectroscopy-William Kemp
- 6. Spectroscopy of organic compounds-P S Kalsi
- 7. Elementary organic spectroscopy-Y R Sharma
- 8. Spectrometric identification of organic compounds-R M Silverstein, G C Bassler& T C Morrill
- 9. Handbook of spectroscopy-G Gauglitz& T Vo-Dinh
- 10. NMR spectroscopy explained-Neil E Jacobsen
- 11. NMR spectroscopy-Joseph B Lambert & Eugene P Mazzolla
- 12. High resolution NMR techniques in organic chemistry-Timothy D W Claridge
- 13. Introduction to Spectroscopy-Pavia Lampman Kriz
- 14. NMR in Chemistry-A multinuclear introduction-William Kemp
- 15. Spectroscopy of organic compounds-P S Kalsi

IPCH-7.2T: ADVANCED ORGANIC SYNTHESIS (Units: 5, Hours: 60, Credits: 4)

Unit-I: Synthetic Strategies-I

Introduction, terminology-target, synthon, synthetic equivalent; functional group inter conversion (FGI), functional group addition, functional group elimination; criteria for selection of target; linear and convergent synthesis; retrosynthesis analysis and synthesis involving chemoselectivity, regioselectivity, reversal of polarity, cyclizations; order of events in synthesis by retrosynthetic approach, explanation by taking examples Salbutamol, Propoxycaine and Dinocap; introduction to one group C-C and C-X disconnections; one group C-C disconnections- alcohols, carbonyl compounds, ethers and sulphides

Unit-II: Synthetic Strategies-II

Introduction to two group C-C and C-X disconnections; two group C-X disconnections-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, Robinson annulations; control in carbonyl condensations, explanation by taking examples oxanamide and mevalonic acid; strategic bond-definition, choosing disconnection/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; other approaches to retrosynthesis-biomimetic approach (Johnsons polyene cyclisation), and retro mass spectral fragmentation; application of the strategies to the synthesis of (+) Disparlure, Retronecine and Longifoline

Unit-III: Principles of Asymmetric Synthesis

Introduction, terminology-topicity in molecules, homotopic, enantiotopic and diastereotopic groups and faces-symmetry, substitution and addition criteria; prochirality, nomenclature-Pro-R, Pro-S, Re and Si faces; stereoselectivity (enantioselectivity and diastereoselectivity), stereospecificity (enantiospecific and diastereospecific); conditions for stereoselectivity-symmetry, transition state criteria, kinetic and thermodynamic control; methods for inducing enantio and diastereoselectivity; analytical methods and techniques for measuring %enantiomeric excess (%ee), %diastereomeric excess (%de), and optical purity-specific rotation, chiral NMR (Chiral derivatizing agents, Chiral solvents, Chiral shift reagents) and Chiral HPLC

Unit-IV: Methodologies in Asymmetric Synthesis

Strategies in asymmetric synthesis-classification

- a). Chiral substrate controlled asymmetric synthesis: Nucleophilic additions to chiral carbonyl compounds; 1,2-asymmetric induction, Cram's rule and Felkin-Anh model
- b). Chiral auxiliary controlled asymmetric synthesis: α -Alkylation of chiral enolates, aza enolates, imines and hydrazones; 1,4-asymmetric induction and Prelog's rule; use of chiral auxiliaries in Diels-Alder reaction.
- c). Chiral reagent controlled asymmetric synthesis: asymmetric reductions using BINAL-H; asymmetric hydroboration using IPC2BH and IPCBH2
- d). Chiral catalyst controlled asymmetric synthesis: Sharpless and Jacobsen asymmetric epoxidations; Sharpless asymmetric dihydroxylation; Asymmetric hydrogenations using chiral Wilkinson biphosphine and Noyori catalyst; Enzyme mediated enantioselective synthesis

e). Asymmetric Aldol reaction: Diastereoselective Aldol reaction (chiral enolate & achiral aldehydes and achiral enolate & chiral aldehydes) its explanation by Zimmerman-Traxel model.

Unit-V: Organometallic Reagents

Organometallic Reagents

Preparation and application of the following organometallic reagents in organic synthesis:

- a) Organo Lithium
- b) Organo Magnesium
- c) Organo Copper
- d) Organo Zinc
- e) Organo Tin
- f) Organo Boranes synthesis and their applications (carbonylation, oxidation, protonolysis)
- g) Organo Silicon reagents (β-carbocations & α-carbanions, Peterson's olefination), TMS halides, TMS cyanides and TMS triflates in organic synthesis
- h) Titanium-Carbene mediated olefination: Tebbe reagent and Petasis reagents

- 1. Organic synthesis-the disconnection approach-S Warren
- 2. Organic synthesis-C Willis and M Willis
- 3. Problems on organic synthesis-Stuart Warren
- 4. Stereochemistry of organic compounds: Principles & Applications-D Nasipuri
- 5. Stereochemistry of carbon compounds-Ernest L Eliel & Samuel H Wilen
- 6. Stereochemistry: conformation & mechanism-P S Kalsi
- 7. The third dimension in organic chemistry-Alan Bassendale
- 8. Stereoselectivity in organic synthesis-R S Ward
- 9. Asymmetric synthesis-Nogradi
- 10. Asymmetric organic reactions-J. D. Morrison and H. S. Moscher
- 11. Principles in asymmetric synthesis-Robert E Gawley & Jeffry Aube
- 12. Stereodifferentiating reactions-Izumi
- 13. Organometallic chemistry and catalysis-Didier Astruc

IPCH-7.3T: MEDICINAL CHEMISTRY-I (Units: 5, Hours: 60, Credits: 4)

Classification, mechanism of action, uses, structural features, significance of ADME properties of drugs mentioned in the course, structure activity relationship (SAR) of selective class of drugs superscripted with (*)

Unit-I: Anti-infective Agents-I

Antibacterial agents: Introduction, drugs acting against cell metabolism: *Sulphonamides, other antimetabolites; drugs inhibiting cell wall synthesis: *Penicillins, *Cephalosporins, β-Lactamase inhibitors and other drugs; drugs acting on the plasma membrane structure: Valinomycin and Gramicidin A and Polymyxin B; drugs impair protein synthesis: translation (Amino glycosides, *Tetracyclines, Chloramphenicol, Macrolides and Oxazolidinones); agents that act on nucleic acid transcription and replication (*Quinolones and fluoroquinolones, *aminoacridines, Rifamycins, nitroimidazoles and nitrofurantoin, inhibitors of bacterial RNA polymerase); miscellaneous agents and drug resistance

Unit-II: Anti-infective Agents-II

Antimalarials: Introduction, *Quinolines: Quinine sulphate, Chloroquine, Amodiaquine, Primaquine phosphate, Pamaquine, Quinacrine hydrochloride and Mefloquine; biguanides; dihydro triazines: Cycloguanil and Proguanil; miscellaneous: Pyrimethamine, Artesunete, Artemether and Atovoquone; Antitubercular agents: Introduction, synthetic anti tubercular agents: Isoniazid, Ethionamide, Ethambutol, Pyrazinamide and p-amino salicylic acid; antitubercular antibiotics: Rifampicin, Rifabutin, Cycloserine, Streptomycin, Capreomycin sulphate and Dapsone; Urinary tract anti-infective agents: *Quinolones: Nalidixic Acid, Norfloxacin, Enoxacin, Ciprofloxacin, Ofloxacin; miscellaneous: Furazolidine, Nitrofurantoin and Methanamine

Unit-III: Anti-infective Agents-III

Leprostatic drugs: Clofazimine, Dapsone, Rifampin and Thalidomide; Antifungal agents: Antifungal antibiotics: Amphotericin-B, Nystatin, Natamycin and Griseofulvin; synthetic antifungal agents: Clotrimazole, Econazole, Butoconazole, Oxiconazole, Tioconozole, *Miconazole, Ketoconazole, Terconazole, Itraconazole, Fluconazole and Tolnaftate; Antiprotozoal Agents: *Metronidazole, Tinidazole, Ornidazole, Diloxanide, Iodoquinol, Pentamidine Isothionate, Atovaquone and Eflornithine; Anthelmintics: Diethylcarbamazine citrate, Thiabendazole, *Mebendazole, Albendazole, Niclosamide, Oxaminoquine, Praziquantal and Ivermectin

Unit-IV: Antiviral Agents

Introduction to viral diseases, antiviral drugs used against DNA viruses: inhibitors of viral DNA polymerase (*Acyclovir, Ganciclovir, Desciclovir, Idoxuridine, Vidarabine, Penciclovir and Foscarnet), inhibitors of tubulin polymerization (Podophyllotoxin), antisense therapy (Fomivirsen); antiviral drugs acting against RNA viruses (HIV): inhibitors of viral reverse transcriptase (Nucleoside inhibitors-Didanosine, *Zidovudine, Lamivudine, Emtricitabine; Non-nucleoside inhibitors-Delavirdine, Nevirapine, Abacavir, Stavudine, Tenofovir, Zalcitabine); Protease inhibitors-*Saquinavir, Indinavir, Nelfinavir and Palinavir; Integrase inhibitor-Raltegravir; antiviral drugs used against RNA virus (Flu): Adamantane and carbocyclic analogues; broad-spectrum antiviral agents: Ribavirin

Unit-V: Anticancer agents

Introduction, drugs acting on enzymes: Methotrexate, 5-Fluro Uracil, Capecitabine, Raltitrexed, Cytarabine, Gemcitabine, *6-Mercaptopurine, Pentostatin and 6-Tioguanine; drugs acting directly on nucleic acids: Dactinomycin, Doxorubicin, Daunorubicin, Mitoxantrone, Amsacrine, Podophyllotoxin, Camptothecin, *Nitrogen mustards, Cyclophosphamide, Chlorambucil, Estramustine and Cisplatin; Hormone-based therapies: Prednisolone, Ethinylestradiol, Diethyl stilbesterol, Fosfestrol, Medroxyprogestesterone acetate, Fluoxmesterone, Testosterone propionate, Leuprolide, goserelin, Tamoxifen, Raloxifene, Toremefene, Fulvestrant, Flutamde, Cyproterone acetate, Abiraterone, Aminoglutethimde, Anastrozole, Letrazole, Formesterone and Mitotane; drugs acting on structural proteins: *Vincistine, Vinblastine, Vindesine, Podophyllotoxin, Maytasine, Combrestatins, epothilones; drugs acting on signaling pathways: L739750, AZD-3409, Lonafarnib, Getitnib, Erlotinib, Imatinib, Sorafenib, Sunitinib, Flavopiridol, Romidepsin, Vorinostat, Revlimid and Actimid

- 1. An introduction to medicinal chemistry-Graham L Patrick, 1st edition
- 2. An introduction to medicinal chemistry-Graham L Patrick, 5th edition
- 3. Foye's principles of medicinal chemistry, 7th edition
- 4. Medicinal chemistry, an introduction-Gareth Thomos, 2nd edition, Wiley Publications

IPCH-7.4T: BIOINORGANC AND PHYSICAL CHEMISTRY (Units: 5, Hours: 60, Credits: 4)

Unit- I: Bioinorganic Chemistry

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: Haemoglobin and Myoglobin, geometric, electronic and magnetic aspects of dioxygen binding, Oxygen adsorption isotherms and co-operativity in Haemoglobin and its physiological significance, role of globin chain; Hemerythrin and Hemocyanin: structure of deoxy forms, oxygen binding, geometric, electronic and magnetic aspects; comparison of Hemerythrin and Hemocyanin with haemoglobin; 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 transamination, decarboxylation and dealdolation in presence of metal ions; Bio-catalysis: Enzyme analogue catalysis, examples of important enzymatic conversions of some >C=O and >C=C< Bonds; artificial enzyme mimics, and catalytic antibodies

Unit-II: Metal Complexes of Small Molecules

Metal nitrosyls: NO as a ligand, molecular orbitals of NO, donor and acceptor components, bonding models of NO-terminal (Linear, Bent) and bridging; structural aspects of $[IrCl(PPh_3)_2(CO)(NO)]^+$ and $[RuCl(PPh_3)_2(NO)_2]^+$; stereochemical control of valance in $[Co(diars)_2(NO)]^{2+}$ and $[Co(diars)_2(NO)(SCN)]^+$; metal dinitrogen complexes: N_2 as a ligand, molecular orbitals of N_2 , bonding models-terminal and bridging, stretching frequencies, structure of Ru(II) and Mo(0) dinitrogen complexes, chemical fixation of dinitrogen; homogeneous catalysis and biocatalysis by metal complexes of small molecules and their catalytic cycles

Unit-III: Electrochemistry-III

Concept of activity and activity coefficients in electrolytic solutions, the mean ionic activity coefficient, Debye-Huckel theory of electrolytic solutions, Debye-Huckel limiting law (derivation not required), calculation of mean ionic activity coefficient from equilibrium constant and solubility product, limitation of Debye-Huckel theory and extended Debye-Huckel law, derivation of Debye-Huckel-Onsager-its validity and limitations; concept of ion association-Bjerrum theory of ion association (elementary treatment) and thermodynamics of ion pairing

Unit-IV Electro Analytical Techniques

Polarography-dropping mercury electrode, instrumentation, Polarogram; types of currents: residual current, limiting current and diffusion current; Ilkovic Equation (derivation not necessary) and its significance; half wave potential and its significance; Fick's first law of diffusion and applications of Polarography; Amperometric titrations: principles, technique involved and applications; Cyclic Voltammetry: principle and applications of Cyclic Voltammetry

Unit-V: Chemical Kinetics

Theories of reaction rates, collision theory, steric factor; transition state theory, reaction coordinate, activated complex and the transition state, thermodynamic formulation of transition state theory, activation parameters and their significance; the Eyring equation; unimolecular reactions and Lindamann's theory; theory of absolute reaction rates; comparison of results with Eyring and Arrhenius equations; ionic reactions and salt effect

- 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
- 4. Advanced physical chemistry-Gurdeep Raj
- 5. Physical chemistry-W J Moore
- 6. Modern electrochemistry 2A & 2B-J O M Bockris & A K N Reddy; Plenum Publishers
- 7. Introduction to electrochemistry-S Glasstone
- 8. Chemical kinetics-K J Laidler; McGraw Hill
- 9. Kinetics and mechanism of chemical transformations-J Rajaraman and J Kuriacose; McMillan

IPCH-7.2LAB: MIXTURE SEPARATION AND IDENTIFICATION OF ORGANIC COMPOUNDS

(Credits: 2, 6hrs/week)

Mixture separation and identification of given organic compounds

Separation and identification of two component mixtures (minimum of 10 mixtures should be separated and analyzed) by chemical methods/reactions: separation by using solvent ether, 5% aqueous sodium bicarbonate, 5% sodium hydroxide and dil. hydrochloric acid, check 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 group tests, preparation of crystalline derivatives and identification by referring to literature standard

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

- 1. Textbook of practical organic chemistry-A I Vogel, A R Tatchell, B S Furnis, A J Hannaford & P W G Smith, Prentice-Hall, 5th edition (1996)
- 2. Practical organic chemistry- F G Mann & B C Saunders, Orient-Longman (1960)
- 3. Comprehensive practical organic chemistry-V K Ahluwalia & R Aggarwal

IPCH-7.3LAB: MEDICINAL CHEMISTRY LAB (Credits: 2, 6hrs/week)

Synthesis, property profiling, SAR and bioavailability of following drugs, in comparison with their close analogues

- 1. Paracetamol
- 2. Phenytoin
- 3. Benzocaine
- 4. Sulfanilamide
- 5. 6-Methy uracil
- 6. Fluorescein
- 7. Phenobarbital
- 7. I licilodaron
- 8. Antipyrine
- 9. Isoniazid
- 10. Dapsone
- 11. Metronidazole
- 12. Curcumin
- 13. Quinine
- 14. Piperine
- 15. Caffeine

- 1. Textbook of Practical Organic Chemistry-A I Vogel, A R Tatchell, B S Furnis, A J Hannaford & P W G Smith, Prentice-Hall, 5th edition (1996)
- 2. Practical Organic Chemistry- F G Mann & B C Saunders, Orient-Longman (1960)
- 3. Comprehensive Practical Organic Chemistry-V K Ahluwalia & R Aggarwal

IPCH-7.4LAB: INORGANIC AND PHYSICAL CHEMISTRY (Credits: 2, 6hrs/week)

Inorganic Chemistry

Preparations:

- 1. Preparation of tris(ethylenediammine)nickel(II)thiosulphate
- 2. Preparation of tetraammine copper(II)sulphate
- 3. Preparation of tris(acetylacetanato)manganese(III)
- 4. Preparation of mercury tetrathiocyanato cobaltate(II)
- 5. Preparation of pentaammine(chloro)cobalt(III)chloride
- 6. Preparation of hexaammine nickel(II)chloride
- 7. Preparation of sodium tris oxalato ferrate(VI)

Estimations:

- 1. Estimations of Ni⁺² by back titration
- 2. Estimation of Ca⁺² by substitution method

Physical Chemistry

- 1. To study the kinetics of saponification of ethyl acetate by NaOH conductometrically
- 2. Determination of mean ionic activities in zinc chloride solutions
- 3. Determination of the mean ionic activity coefficients hydrochloric acid solutions at different concentrations

- 1. Textbook of Practical Organic Chemistry-A I Vogel, A R Tatchell, B S Furnis, A J Hannaford & P W G Smith, Prentice-Hall, 5th edition (1996)
- 2. Practical Organic Chemistry- F G Mann & B C Saunders, Orient-Longman (1960)
- 3. Comprehensive Practical Organic Chemistry-V K Ahluwalia & R Aggarwal

SEMESTER-VIII

IPCH-8.1T: PHARMACEUTICAL CHEMISTRY

(Units: 5, Hours: 60, Credits: 4)

Unit-I: Significance of Purity, Integrity and Optimization of Solubility

Significance and effects of purity and integrity of lead molecule; fundamentals of solubility, effect of solubility, effects of physiology on solubility and absorption, effect of pH on the solubility of acidic and basic drugs, structure modification strategies to improve solubility, strategies for improving dissolution rate; salt form: solubility of salts, effect of salt form on absorption and oral bioavailability, salt selection, precautions for using salt forms, case studies of structure modification strategies for improving solubility, case studies on salt formation to improve solubility

Unit-II: Optimization of Lipophilicity, pKa and Permeability

Lipophilicity fundamentals, effects of lipophilicity, partition coefficient, practical and theoretical determination of partition coefficients, case studies on structure modifications to optimize lipophilicity; pKa fundamentals, effects of pKa, case studies on structural modifications to optimize pKa; fundamentals of permeability, effects of permeability, structure modification strategies to modify permeability

Unit-III: Optimization of BBB Penetration and Metabolic Stability

BBB fundamentals, effect of brain penetration, structure and BBB penetration, structure modification strategies to improve brain penetration; metabolic stability: effects of metabolic stability, structure modification strategies to improve phase-I and II metabolic stability, consequences of chirality on metabolic stability, substrate specificity on CYP isozymes, CYP inhibition fundamentals, effect of CYP inhibition, structure modification strategies to reduce CYP inhibition

Unit-IV: Plasma Stability, Solution Instability, Plasma Protein Binding

Plasma stability fundamentals, effect of chirality on plasma stability, effect of plasma stability, structural modifications to improve plasma stability, applications of plasma stability data; solution stability: solution stability fundamentals, effect of solution instability, structure modification strategies to improve solution stability, applications of solution stability data; plasma protein binding: fundamentals of plasma protein binding, effect of chirality on plasma protein binding, effect of protein binding, structure modification strategies for plasma protein binding

Unit-V: Drug Delivery Approach to Improve Solubility, Bioavailability and Safety Profile Formulation methods to improve water solubility, introduction and pharmaceutical applications of cosolvents, colloidal solutions, emulsions, drug solubilisation through surfactants and amphiphiles, micelles, liposomes and nanoparticles as drug delivery systems (particle technology for solubility); toxicity fundamentals, toxicity terms and mechanisms, structure modification strategies to avoid toxicity, case studies of toxicity of drugs

- 1. An introduction to medicinal chemistry-Graham L Patrick, 1st edition
- 2. An introduction to medicinal chemistry-Graham L Patrick, 5th edition
- 3. Foye's principles of medicinal chemistry, 7th edition
- 4. Medicinal chemistry, an introduction-Gareth Thomos, 2nd edition, Wiley Publications
- 5. Drug like properties: concept, structure design and methods (from ADME to toxicity optimization), Edward H Kerns & Li Di, Academic press, Elsevier publications

Syllabus for 5yrs Integrated M.Sc Chemistry (Pharmaceutical Chemistry), Effective from AY 2015-16 Department of Pharmaceutical Chemistry, Telangana University, Dichpally, Nizamabad-503322

- 6. The practice of medicinal chemistry-Camille Georges Wermuth, 2nd/3rd/4th edns, Academic press, Elsevier publications
- 7. Principles of medicinal chemistry- William O Foye, B I Waverly Pvt. Ltd, New Delhi
- 8. Burger's medicinal chemistry, Walffed John Willey and Sons, Wiley-Inter Science Publication, New York, Toranto

IPCH-8.2T: HETEROCYCLIC CHEMISTRY

(Units: 5, Hours: 60, Credits: 4)

Unit-I: Three and Four Membered Heterocycles

Nomenclature of heterocyclic systems based on ring size, number and nature of hetero atoms; different types of strains, interactions and conformational aspects of non aromatic heterocycles; synthesis, reactivity, stability and pharmaceutical importance of the following ring systems: aziridine, azirine, oxirane, thiirane; azetidine, oxetane, thietane; diazirines, diaziridines, oxaziridines

Unit-II: Five Membered Heterocycles-I

Synthesis, aromaticity, reactivity and pharmaceutical importance of pyrrole, furan, thiophene; indole, benzofuran, benzothiophene; imidazole, pyrazole; oxazole, isoxazole; thiazole, isothiazole; benzimidazole, benzoxazole, benzthiazole; carbazole

Unit-III: Five Membered Heterocycles-II

Synthesis, aromaticity, reactivity and pharmaceutical importance of 1,2,3-triazole, 1,2,4-triazole; Sydnones (1,2,3-oxadiazole), 1,2,5-oxadiazole; 1,2,3-thiadiazole, 1,2,4-thiadiazole; tetrazole; benzotriazole; selenophenes, tellurophenes, phospholes, boroles

Unit-IV: Six Membered Heterocycles

Synthesis, aromaticity, reactivity and pharmaceutical importance of pyran, piperidine, pyridine; quinoline, isoquinoline; acridine; pyridazine, pyrimidine, pyrazine; oxazine, thiazine; 1,2,3-triazine, 1,2,4-triazine, 1,3,5-triazine; 1,2,4,5-tetrazine; coumarin, chromone, pteridine

Unit-V: Larger Ring (>6) and Other Heterocycles

Synthesis and reactivity of azepine, oxepine, thiepine; benzoazepine, benzooxepine, benzothiepine; 1,3-benzodiazepine, 1,4-benzodiazepine, 1,5-benzodiazepine; azocine; azonine; quinolizine, imidazopyridine; purines, xanthine, caffeine, theobromine, theophylline, uric acid

- 1. The chemistry of heterocycles-Theophil Eicher & Siegfried Hauptmann
- 2. Heterocyclic chemistry-T Gilchrist
- 3. An introduction to the chemistry of heterocyclic compounds-R M Acheson
- 4. Principles of modern heterocyclic chemistry-A Paquette
- 5. Handbook of heterocyclic chemistry-A R Katritzky
- 6. Microwave assisted synthesis of heterocycles-Eric Van Der Eycken and Oliver Kappe
- 7. Heterocycles from carbohydrate precursors-El Sayed H & El Ashry
- 8. Heterocyclic antitumor antibiotics-Moses Lee
- 9. Heterocyclic chemistry-M Sainsbury
- 10. Heterocyclic chemistry (4 Edn)-John A Joule, Keith Mills & George Smith
- 11. Heterocyclic chemistry (5 Edn)-John A Joule & Keith Mills
- 12. Aromaticity in heterocyclic compounds-Tadeusz M Krygowski & Michał K Cyranski
- 13. Handbook of heterocyclic chemistry (2 Edn)-Alan R Katritzky & Alexander F Pozharskii
- 14. Handbook of heterocyclic chemistry (3 Edn)-Alan R Katritzky
- 15. Name reactions in heterocyclic chemistry-Jie Jack Li
- 16. Progress in heterocyclic chemistry-Gordon W Gribble & John A Joule

IPCH-8.3T: MEDICINAL CHEMISTRY-II (Units: 5, Hours: 60, Credits: 4)

Study of the development of the following classes of drugs, Classification, mechanism of action, uses of drugs, significance of ADME properties of drugs mentioned in the course, Structure activity relationship of selective class of drugs superscripted with (*)

Unit-I: Drugs Acting on Autonomic Nervous System

Drugs acting on cholinergic system: cholinergic agonists, structure, structure activity relationships and receptor binding of ACh, muscarinic antagonists, antagonists of nicotinic cholinergic receptors, anticholinesterase drugs: carbamates, organophophorous compounds; pralidoxime as antidote, anticholinesterases as 'Smart Drugs'.

Drugs acting on adrenergic system: adrenergic agonists, adrenergic antagonists, SAR, other drugs affecting adrenergic transmission: drugs that affect the biosynthesis of adrenergics, drugs inhibit the uptake of noradrenaline into storage vesicles, drugs affecting release of noradrenaline from storage vesicles, reuptake inhibitors of noradrenaline into presynaptic neurons, drugs inhibiting metabolic enzymes

Unit-II: Drugs Acting on Central Nervous (CNS) System

CNS depressants: anxiolytic, sedative and hypnotic agents; *benzodiazepines and related compounds, *barbiturates, miscellaneous (amides, imides, alcohols and their carbamates, aldehydes and their derivatives) antipsychotics; *phenothiazines, *fluorobutyrophenones; antimaniac agents; lithium salts, anticonvulsant drugs

CNS stimulants: antidepressants; monoamine oxidase inhibitors (MAOIs), mono amine reuptake inhibitors, *tricyclic antidepressants (TCAs), selective Serotonin reuptake inhibitors (SSRIs), analeptics

Treatment of CNS degenerative disorders: anti-Parkinsonian agents and anti-Alzheimer's agents

Unit-III: Drugs Acting on Cardiovascular System and Analgesic Agents

Cardiovascular agents: antianginal agents and vasodilators; antiarrhythmic agents; anti hypersensitive agents; anticoagulants

Opioid analgesics: analogues of *morphine, opioid agonists and antagonists; anti-inflammatory analgesics (NSAIDs): salicylic acid derivatives, N-anthranilic acid derivatives, *arylacetic acid derivatives, aniline and p-aminophenol derivatives, other NSAIDs

Unit-IV: Drugs Acting on GIT and Renal System

Drugs acting on GIT: antiulcer agents; H₂ antagonists, proton pump inhibitors, antiemetic agents Drugs acting on renal system: diuretics; introduction, carbonic anhydrase inhibitors, *thiazide and thiazide like diuretics, loop diuretics, potassium sparing diuretics, miscellaneous diuretics, angiotensin converting enzyme inhibitors, design of angiotensin converting enzyme inhibitors

Unit-V: Drugs Acting on Endocrine Glands and Anesthetics

Antidiabetics, Thyroid and Antithyroid drugs

Steroid hormones; steroid nomenclature, stereochemistry and numbering, estrogen and antiestrogen products, progestin products, androgen and antiandrogen products, aldosterone antagonists, mineralocorticoids and glucocorticoid products, chemical contraceptive agents

Anesthetics: general anesthetics; inhalational anesthetics, intravenous anesthetics; local anesthetics; *ester-based local anesthetics, *amide-based local anesthetics, miscellaneous compounds with local anesthetic activity

- 1. Wilson and Gisvold's Text book of organic, medicinal and pharmaceutical chemistry, Lippincott-Raven Publishers-New York, Philadelphia
- 2. Principles of medicinal chemistry-William O Foye, B I Waverly Pvt. Ltd., New Delhi
- 3. Burgers' medicinal chemistry, Walffed John Willey and Sons, Wiley-Interscience Publication, New York, Toranto
- 4. Pharmacology- Rang H P and Dale M M, Churchill Living Stone publisher, 4th edn, 1999
- 5. Gilman's the pharmacological basis of therapeutics- Goodman Gilman A, Rall T W, Nies A I S & Taylor P Goodman, Mc Graw Hill publishers, Pergamon press, 9th edn, 1996
- 6. A text book of medicinal chemistry (Vol-I&II)-Surendra N Pandey, S G Publishers, Varanasi
- 7. Indian pharmacopoeia 1985 and 1996, the controller of publications, civil lines, Delhi
- 8. Current Index of Medical Specialities (CIMS) and MIMS India, MIMS, A.E. Morgan publications (I) Pvt. Ltd, New Delhi
- 9. The science and practice of pharmacy (Vol-1&2)-Remington, MACK publishing company, Easton, Pennsylvania

IPCH-8.4T: PHYSICAL AND GENERAL CHEMISTRY (Units: 5, Hours: 60, Credits: 4)

Unit-I: Chemistry of Materials

Classification of materials-metals, ceramics, polymers, composites, semiconductors, biomaterials and their properties; preparative methods of solid materials: co-precipitation, sol-gel process, high pressure and hydrothermal methods, arc techniques and other useful techniques; application of materials in science and technology including pharmacy; techniques of single crystal growth, growth from solutions, growth from melts, growth from vapour; non linear optical materials-basic concepts with examples; liquid crystals-basic concepts with examples and their typical applications; thermal sensitivity of the materials and useful thermal analysis characterization techniques (TGA & DSC) of materials

Unit-II: Medicinal Inorganic Chemistry

Metal ion binding sites present in amino acids, peptides, proteins, enzymes, nucleoside and nucleotide; interactions of metal ion and metal complexes with the biomolecules, basics of apo-enzymes and metalo enzymes; metal ion toxicity in humans and animals; detoxifications using chelating agents (Chelation therapy); inorganic compounds used as drugs and diagnostic agents: metal based anticancer drug Cis Pt(NH3)2Cl2 and its mode of action, gold-containing drugs used in therapy of Rheumatoid arthritis, therapeutic agent for Menkes disease; copper-histidine anti viral chemotherapy and metal peptide interactions; drug binding DNA cleavage pathways of metal complexes; role of metal ions in the action of antibiotics-with examples; transition and main element based diagnostic and therapeutic radiopharmaceuticals

Unit-III: Symmetry Properties of Molecules and Group Theory

Concept of symmetry in chemistry, symmetry operations, symmetry elements: rational axis of symmetry and types of rational axes, plane of symmetry and types of planes, improper rational axis of symmetry, inversion centre and identity element; more about symmetry elements-molecular point groups: definition and notation of point groups, classification molecules into C_1 , C_s , C_i , C_n , C_{nv} , C_{nh} , $C_{\alpha v}$, D_n , $D_$

Unit-IV: Thermodynamics and Chemical Kinetics

Third law of thermodynamics and determination of absolute entropies of solids, liquids and gases-problems; complex reactions-opposing reactions, parallel reactions and consecutive reactions (all first order type); steady state treatment; example of $H_2 - Br_2$ reaction; derivation of rate law; effect of structure on reactivity: linear free energy relationships; Hammett and Taft equations-substituent (σ and σ^*) and reaction constant (ρ and ρ^*) with examples; deviations from Hammett correlations, reasons; change of mechanism, resonance interaction; Taft four parameter equation; correlations for nucleophilic reactions; the Swain-Scott equation and the Edward equation; reactivity: selectivity principle and the isoselectivity rule; the intrinsic barrier and Hammond's postulate; kinetics of photochemical reactions and free radical polymerization

Unit-V: Quantum Chemistry

Particle in a box: one dimensional; plots of \Box and \Box^2 -discussion; degeneracy of energy levels; comparison of classical and quantum mechanical particles; calculations using wave functions of the

particle in a box: orthogonality, measurability of energy, position and momentum, average values and probabilities; application to the spectra of conjugated molecules; cartesian, polar and spherical polar coordinates and their interrelations and particle in a three dimensional box; Schrodinger equation for the hydrogen atom: separation into three equations-hydrogen like wave functions, radial and angular functions, 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, H₂⁺ ion, the variation integral for H₂⁺ 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 H₂ molecule MO by LCAO method and Valence bond method (detailed calculations not required); comparison of MO and VB models

- 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
- 4. Molecular thermodynamics-D A McQuarrie and J D Simon, University Science Books
- 5. Quantum chemistry-Ira N Levine, Prentice hall
- 6. Chemical kinetics-K J Laidler, McGraw hill
- 7. Kinetics, mechanism and chemical transformations-J Rajaraman and J Kuriacose, McMillan
- 8. Chemical kinetics and reaction mechanisms-J H Espenson, McGraw Hill
- 9. Physical organic chemistry-N S Isaacs, ELBS

IPCH-8.1LAB: ORGANIC CHEMISTRY LAB (Credits: 2, 6hrs/week)

A minimum of 7-10 compounds from the following list should be prepared. In the lab work, focus should be on stoichiometric calculations, mechanism, synthesis, purification and analysis

2-Phenyl indole (Fischer indole synthesis), 2,5-dihydroxy acetophenone (Fries reaction), benzilic acid from benzoin (rearrangement), benzpinacol (photochemical reaction), 7-hydroxy coumarin (Pechman synthesis), benzanilide (Beckmann rearrangement), phenytoin, antipyrine, 7-hydroxy-3-methyl flavone (Baker-Venkatraman reaction), photo-dimerization of maleic anhydride, benzophenone (Friedel-Crafts reaction), acridone from phthalic anhydride, benzocaine, quinoline (Skraup synthesis), 1-phenyl-3-methyl-5-pyrazole, Vanillyl alcohol from vanillin (using NaBH₄), 5-hydroxy-1,3-benzoxazol-2-one, 1,2-diphenyl-5-nitrobenzimidazole, 4-iodonitrobenzene (Sandmeyer reaction), 2-chlorobenzoic acid

- 1. Laboratory manual of organic chemistry-Raj K Bansal
- 2. Textbook of practical organic chemistry-Vogel A I, Tatchell A R, Furnis B S, Hannaford A J & Smith P W G, Prentice-Hall, 5th edition (1996)
- 3. Practical organic chemistry-Mann F G & Saunders B C, Orient-Longman (1960)
- 4. Comprehensive practical organic chemistry- Ahluwalia V K & Agarwal R

IPCH-8.2LAB: SPECTROSCOPY LAB (Credits: 2, 6hrs/week)

Identification of Organic Compounds by Spectral Methods

Structure determination of unknown organic compounds by interpretation of IR, UV, 1HNMR, 13CNMR and Mass spectral data and a minimum of 15 representative examples should be studied.

Reference Books

Spectroscopic identification of organic compounds-Silverstein, Bassler and Morril, 5th Edn

IPCH-8.3LAB: PHARMACEUTICAL CHEMISTRY LAB-I (Credits: 2, 6hrs/week)

- 1. Experimental determination of partition coefficient, pKa, solubility of various drugs
- 2. Preparation and evaluation of Paracetamol suspension in comparison with tablets
- 3. Preparation and evaluation of curcumin nanoparticles in comparison with curcumin tablets
- 4. Preparation and evaluation of liposomes of few drugs
- 5. Preformulation studies of few bulk drugs
- 6. Experiments investigating the permeability of drugs through BBB and plasma membrane
- 7. Experiments for determination of solution stability and plasma stability of drugs
- 8. Experiments demonstrating effect on solubility and permeability by various analogues of a drug

- 1. An introduction to medicinal chemistry-Graham L Patrick, $\mathbf{1}^{\mathrm{st}}$ edn
- 2. An introduction to medicinal chemistry-Graham L Patrick, 5th edn
- 3. Foye's principles of medicinal chemistry, 7th edn
- 4. Medicinal chemistry, an introduction-Gareth Thomos, 2nd edn, Wiley Publications

SEMESTER-IX

IPCH-9.1T: PERICYCLIC AND PHOTO CHEMISTRY

(Units: 5, Hours: 60, Credits: 4)

Unit-I: Pericyclic Reactions-I

Introduction, features and classification of pericyclic reactions; molecular orbital phases, nodes and symmetry properties of ethylene, 1,3-butadiene, 1,3,5-hexatriene, allyl cation, allyl radical, pentadienyl radical and pentadienyl cation

Electrocyclic Reactions: Ring opening and ring closure in 4n and 4n+2 systems, conrotatory and disrotatory motions; Woodward-Hoffmann selection rules; analysis of reaction mechanism by Orbital Correlation Diagrams, Frontier Molecular Orbital (FMO) method and Aromatic Transition State (ATS) method (Huckel-Mobius Transition State theory)

Unit-II: Pericyclic Reactions-II

Cycloaddition Reactions: Cycloadditions in 2+2 and 4+2 systems, cycloreversions, stereochemical aspects of suprafacial (supra), antarafacial (antara) interactions; Diels-Alder reaction and Exo-Endo selectivity; 1,3-dipolar cycloadditions; Woodward-Hoffmann selection rules; analysis of reaction mechanism by Orbital Correlation Diagrams, Frontier Molecular Orbital (FMO) method and Aromatic Transition State (ATS) method (Huckel-Mobius Transition State theory)

Chelotropic Reactions and Group Transfer Reactions (Ene reaction)

Unit-III: Pericyclic Reactions-III

Sigmatropic Rearrangements: Suprafacial and antrafacial shifts; [1,j] and [i,j] shifts and selection rules; sigmatropic shifts involving carbon moieties, 3,3- and 5,5-sigmatropic rearrangements; analysis of reaction mechanism by Frontier Molecular Orbital (FMO) method and Aromatic Transition State (ATS) method (Huckel-Mobius Transition State theory); Claisen, Cope and oxy-Cope rearrangements **Aromaticity:** Introduction, aromatic, non aromatic, anti aromatic and homo aromatic compounds; Huckel $4n+2\pi$ electron rule, Frost-Musulin diagrams and Craig's rule

Examples: cyclopropene, cyclopropenyl cation, cyclopropenyl anion, cyclopentadienyl cation, cyclopentadienyl anion, benzene, naphthalene, chrysene, Tropylium cation; [8], [10], [12], [14], [16] and [18]-annulenes; azulenes, pentalene, heptalene, triafulvalene, pentafulvalene, tripentafulvalene, heptafulvalene, acenapthylene

Unit-IV: Organic Photochemistry-I

Laws of photochemistry, electronic transitions, Jablonski diagram; singlet, triplet states; photosensitizer; photochemistry of carbonyl compounds: photo reduction, photo cyclo addition (Paterno-Buchi reaction), photo cleavage (Norrish type-I and type-II reactions), photo rearrangement; photochemistry of α,β -unsaturated carbonyl compounds: photo cyclo dimerization, photo cyclo addition; photochemistry of 4,4-disubstitued cyclohexenone and cyclohexadienone

Unit-V: Organic Photochemistry-II

Photochemistry of alkenes: cis-trans isomerization, photo cyclo dimerization, photo cyclo addition, simple addition, intra molecular crossed addition reactions; photochemistry of conjugated dienes: cycloaddition reactions of 1,3-butadiene; photochemistry of 1,4-dienes: di-pi-methane rearrangement; photochemistry of aromatic compounds: photo rearrangement, photo cyclo addition, photo simple addition, photo substitution and photo cyclisation; photo fragmentation reaction (Barton reaction); photooxygenation-formation of dioxetanes, peroxides; photochemistry of azo, diazo, azides and diazonium salts; photobiology: thymine 2+2 cyclo addition, synthesis of vitamin-D

- 1. Pericyclic reactions-a mechanistic study-Mukherjee S M
- 2. Conservation of orbital symmetry-Woodward & Hoffmann
- 3. Organic reactions and orbital symmetry-Gilchrist & Storr
- 4. Pericyclic reactions-a problem solving approach-Lehr & Merchand
- 5. Aromatic character and aromaticity-G M Badger
- 6. Non-benzenoid aromatic compounds-D Ginsberg
- 7. Non-benzenoid compounds-Lloyds
- 8. Pericyclic reactions-a textbook-S Sankararaman, Wiley-VCH, 2005
- 9. Pericyclic reactions-I Fleming, Oxford University Press, 1999
- 10. Modern molecular photochemistry of organic compounds-N J Turro, V Ramamurthy & J C Scaiano, University Science Books, 2010
- 11. Organic chemistry-Clayden, Greeves, Warren & Wothers

IPCH-9.2T: ORGANOMETALLICS, HOMOGENEOUS CATALYSIS & ADVANCED ORGANIC SYNTHESIS-II

(Units: 5, Hours: 60, Credits: 4)

Unit-I: Structure and Bonding in the Organometallics of d-Block Metals

Definition/classification, common ligands used in organometallics and hapticity, 18 electrons rule, popular methods of M-C bond synthesis in transition metal organometallic chemistry, structure and bonding in σ -complexes (with alkyls, aryls and related σ bonding ligands) and π -complexes (with alkenes, alkynes, dienes, allyls, arenes and related unsaturated related ligands) of d-block metals with representative examples; common reactions of organometallics: oxidative addition, reductive elimination, migratory insertion, elimination; modules for OMC reactions; N-heterocyclic carbenes (NHCs): Synthesis, comparison between the structural features of Fischer, Schrock and Arduengo carbenes and the related organometallics, Wanzlick equilibrium

Unit-II: Homogeneous Catalysis-I (non-asymmetric/asymmetric)

General aspects of catalysis in fine, bulk, fuel, polymer, energy, agricultural and environmental process: Industrially demanding homogeneous catalysis by transitions metals and the effect of ligands, catalytic cycles and intermediates of (non-asymmetric/asymmetric processes) Ru(II) catalyzed olefin metathesis, carbonylation (Monsanto process); Rh(I) catalyzed olefin hydrogenation, transfer hydrogenation and hydroformylation (Ruhrchemie/Rhone–Poulenc process); Pd(II) catalyzed Wacker process, cross-couplings and isomerisation of olefins and ligand influence; metal catalyzed cycloaddition (click chemistry in 1,3-dipolar cycloadditions); metallocene catalysis in olefin polymerization; homogeneous catalysis by gold: C-H activation reactions; oligomerization and Shell-Higher-Olefins-Process; homogeneous oxidations, epoxidations and hydroxylations; usefulness of supported homogeneous catalysts with some examples; designing of Tandem/Cascade/Sequential processes in one-pot methodologies

Unit-III: Homogeneous Catalysis-II ((non-asymmetric/asymmetric)

Transition metal complex catalyzed hydrofunctionalization of olefins (hydrocyanation, hydroamination and hydrothiolation, hydrosilylation); Chiral organometallics based catalysis in drug synthesis: enantioselective synthesis-stereoselective catalysis-hydrogenation to L-Dopa, (S)-Ibuprofen, (S)-Naproxen, L-menthol and isomerisation and relevant examples; Organocatalysis: basics of organocatalysts categories (amines, chiral amides, iminium, and NHCs); Organocatalysis by Nheterocyclic carbenes: Reactivity and modes of Action of NHCs in different organocatalysis reactions (Umpolung, Benzoin condensation, Stetter reaction, hydroacylation, enolate transesterification, oxidative NHC catalysis; Metal-Ligand cooperative/synergistic catalysis (asymmetric/non-asymmetric); Agostic interactions in catalysis. Use of kinetics and spectroscopic studies in catalysis

Unit-IV: New Synthetic Reactions

Cross coupling reactions: Suzuki coupling, Stille coupling, Negishi coupling, Kumada coupling, Heck reaction, Sonogashira coupling, Buchwald-Hartwig coupling; Grubb catalysts and cross metathesis (CM), ring closing metathesis (RCM), ring opening metathesis (ROM); McMurrey reaction, Julia-Lythgoe olefination, Peterson olefination, Wittig reaction, Horner-Wodsworth-Emmons reaction, Mukayama Aldol reaction, Baylis-Hillman reaction, Mitsunobu reaction, Shapiro reaction, BINOL and BINAP assisted reactions, Ugi multi component reaction, Mannich reaction, Michael addition, Click reaction

Unit-V: New Techniques and Concepts in Organic Synthesis

Discuss the following techniques in detail and the steps involved in the process like protection and deprotection of various interfering functional groups

Solid phase polypeptide synthesis, solid phase oligonucleotide synthesis, solid phase oligosaccharide synthesis and Kahne glycosidation, combinatorial chemistry, phase transfer catalysis, tandem synthesis, Baldwin rules, chiron approach in organic synthesis: synthesis of Shikimic acid from Darabinose, transformations using esterases and lipases, determination of absolute configuration using Mosher's method

- 1. Basic principles of organic chemistry-John D Robert & Marjorie C Caserio, 2nd edn
- 2. Advanced organic chemistry: reactions, mechanisms & Structure-M B Smith & J March
- 3. Organic chemistry-Clayden, Greeves, Warren & Wothers
- 4. Name reactions and reagents in organic synthesis-Bradford P Mundy, Michael G Ellerd & Frank Favaloro
- 5. Some modern methods of organic synthesis-W Carruthers
- 6. Guide book to organic synthesis-R K Meckie, D M Smith & R A Atken
- 7. Organic synthesis-O House
- 8. Organic synthesis-Michael B Smith
- 9. Organic synthesis-Robert E Ireland
- 10. Organic synthesis-C Willis and M Willis
- 11. Problems on organic synthesis-Stuart Warren
- 12. Name reactions-Jie Jack Li
- 13. Tandem organic reactions-Tse-Lok Ho
- 14. The organometallic chemistry of transition metals- R. H Crabtree, 4th edn, Wiley-VCH, 2005
- 15. Inorganic chemistry, principles of structure and reactivity- J E Huheey, E A Keiter and R L Keiter, 4th edn, Harper Collin College Publishers, 1993
- 16. Organotransition metal chemistry: From bonding to catalysis- J F Hartwig, 1st edn, University Science Books, 2010
- 17. The organometallic chemistry of N-heterocyclic carbenes- Han Vinh Huynh, Wiley-VCH-2017
- 18. Organometallic chemistry-R C Mehrotra, New Age International (P) Limited, 2007
- 19. Organometallic chemistry and catalysis-Didier Astruc, Springer, 2007
- 20. Homogeneous catalysis (Understanding the Art)-P W N M van Leeuwen, Springer, 2004
- 21. N-Heterocyclic carbenes in organocatalysis-Akkattu T Biju

IPCH-9.3T: NATURAL PRODUCTS

(Units: 5, Hours: 60, Credits: 4)

Unit-I: Terpenoids

Introduction, general properties of terpenoids, isolation methods, isoprene rule, special isoprene rule, classification of terpenes, synthesis of hemiterpenoid (isoprene); structure determination and synthesis of acyclic monoterpenoids-Citral, Geraniol; monocyclic monoterpenoids- (α) -Terpineol; bicyclic mono terpenoids-Camphor; monocyclic sesquiterpenoid-Bisabolene; diterpenoid-Abietic acid; triterpenoid-Squalene

Unit-II: Alkaloids

Introduction, classification, isolation methods, general methods of structure elucidation; structure elucidation and synthesis of pyridine-pyrrolidine alkaloid-Nicotine; quinoline alkaloid-Quinine; isoquinoline alkaloid-Papaverine; phenanthrene alkaloid-Morphine; indole alkaloid-Reserpine

Unit-III: Steroids and Hormones

Steroids: Introduction, Diel's hydrocarbon, structure elucidation of Ergosterol and Stigmasterol, stereochemistry and synthesis of Cholesterol

Hormones: Introduction, classification, structure elucidation and synthesis of male sex hormones-Androsterone and Testosterone, structure elucidation and synthesis of female sex hormones-Oestrone and Progesterone

Plant Hormones: Introduction, classification of plant hormones, structure elucidation of Gibberellic acid

Unit-IV: Antibiotics, Prostaglandins and Flavones

Antibiotics: Introduction, characteristics of antibiotics, classification of antibiotics, synthesis of Penicillins, Cephalosporin-C; Streptomycin (Aminoglycoside), Chloramphenicol, Tetracycline

Prostaglandins: Introduction, classification, biological role of prostaglandins, structure elucidation and synthesis of PGE

Flavones-Introduction, classification, structure elucidation and synthesis of Quercetin

Unit-V: Biosynthesis of Natural Products

Introduction, biosynthesis of terpenoids (Menthol and Squalene), biosynthesis of steroids (Cholesterol), biosynthesis of alkaloids (Quinine and Papaverine), biosynthesis of flavonoids, biosynthesis of prostaglandins (PGF); color reactions of natural products; alkaloid degradation methods: Hoffman exhaustive methylation, Emde and von Braun method

- 1. Organic chemistry of natural products-Gurdeep R Chatwal (Vol-I&II)
- 2. Organic chemistry of natural products-O P Agarwal (Vol-I&II)
- 3. Organic Chemistry-I L Finar (Vol-1&2)
- 4. Medicinal natural products-Dewick
- 5. Alkaloids-Manske
- 6. Alkaloids-Pelletier
- 7. Alkaloids-Bentely

IPCH-9.4T: MODERN DRUG SYNTHESIS (Units: 5, Hours: 60, Credits: 4)

Modern drug synthesis provides the platform to students to learn the applications of various reagents, protecting groups and their deprotection, stereochemistry, retrosynthesis, purification and pharmacology in the process of synthesis of various drugs presented here.

Unit-I:

Anticancer Agents: Introduction, synthesis and pharmacology of DNA methyltransferase inhibitor-Decitabine, oral chemotherapy agent-Capecitabine, multi-kinase inhibitor-Soraferib

Antiinfective Agents: Introduction, synthesis and pharmacology of HIV-1 integrase inhibitor-Raltegravir, CCR5 antagonist-Maraviroc, HIV-1 protease inhibitor-Darunavir

Antibacterial Agents: Introduction, synthesis and pharmacology of bacterial DNA gyrase and topoisomerase inhibitor-Ciprofloxacin and protein synthesis inhibitor-Linezolid

Unit-II:

Cardiovascular Agents: Introduction, synthesis and pharmacology of renin inhibitor-Aliskiren, vasopressin V1a and V2 receptor antagonist-Conivaptan, factor-Xa inhibitor-Rivaroxaban

Drugs Acting on Renal Function: Introduction, synthesis and pharmacology of aldosterone antagonist-Spironolactone, renal epithelial Na⁺ channel inhibitor (K⁺ sparing diuretic)-Amiloride

Drugs Acting on Respiratory System: Introduction, synthesis and pharmacology of centrally acting antitussive–Dextromethorphan, peripherally acting antitussive–Caramiphen

Unit-III:

CNS Agents: Introduction, synthesis and pharmacology of $\alpha 4\beta 2$ nicotinic receptor partial agonist-Varenidine, cholinesterase inhibitors-Donepezil, Rivastigmine, Galantamine

Narcotic Analgesics: Introduction, synthesis and pharmacology of μ -opioid receptor agonist-Morphine, μ -receptor antagonist or partial agonist-Pentazocine

Drugs Acting on Hormones: Introduction, synthesis and pharmacology of iodination of thyroglobulin inhibitor-Propylthiouracil, Methimazole and estrogen agonists-Stilbestrol, Dienoestrol

Unit-IV:

Metabolic Diseases: Introduction, synthesis and pharmacology of reversible DPP-4 inhibitor-Sitagliptin, pancreatic β -cell agonist-Tolbutamide, peroxisome proliferator activated receptor- γ (PPAR- γ) agonist-Ciglitazone

Antiulcer Agents: Introduction, synthesis and pharmacology of H₂-receptor antagonist-Cimetidine, proton pump inhibitor-Omeprazole

Antidiarrhoeals: Introduction, synthesis and pharmacology of μ -opioid agonist (adsorbent)-Diphenoxylate, antisecretory agent-Sulphasalazine

Unit-V: Chiral Drugs

Importance of chiral drugs, eutomer, distomer, eudesmic ratio, three point contact model-Pfeiffer's rule; synthesis of dopaminergic agonist L-Dopa, antioxidant (R,R,R)-Tocopherol, calcium channel blocker (2S,3S)-Diltiazem, cyclooxygenase (COX) inhibitors (S)-Ibuprofen and (S)-Naproxen, β adrenergic receptor antagonist Propranolol, angiotensin converting enzyme (ACE) inhibitors Ramipril and Quinapril, HIV-reverse transcriptase inhibitor Lamivudine, H_1 -blocker Fexofenadine

- 1. Modern drug synthesis-Jie Jack Li & Douglas S Johnson
- 2. Contemporary drug synthesis- Jie Jack Li, Douglas S Johnson, Drago R Sliskovic & Bruce D Roth
- 3. The art of drug synthesis- Douglas S Johnson & Jie Jack Li
- 4. Wilson and Gisvold's text book of organic medicinal and pharmaceutical chemistry-John H Block & John M Beale (11th edition)
- 5. Foye's principles of medicinal chemistry-Thomos L Lemke, David A Williams & Lippincott Williams
- 6. Goodman and Gilman's manual of pharmacology and therapeutics, McGraw Hill publications
- 7. Chirality in drug research-Mannhold R, Kubinyi H & Folkers G

9.5T: MOLECULAR MODELLING AND DRUG DESIGN (Units: 5, Hours: 60, Credits: 4)

Unit-I: Molecular Graphics

Introduction to molecular modeling tools, Different graphical representations of molecules (Ball and stick, Wire frame, Licorice, Space fill, Ribbon), molecular surfaces (van der Waal, CPK, solvent accessible surface, solvent excluded surface), molecular Data representation formats (2D, 3D data formats: SDF, CML, SMILES, PDB, GROMACS, CHARMM, SLN, SMARTS, XYZ, MDL Number), QM, MM, Force fields in use, Coordinate systems, Potential energy surface, Energy minimization, software used and applications of molecular graphics.

Unit-II: Molecular Docking

Steps involved in docking, flexible docking, rigid docking, interpretation and applications, Software used, Advantages and disadvantages of docking software with successful examples; Virtual screening, pharmacophore modeling, programs used for pharmacophore generation, Monte Carlo simulations and molecular dynamics in performing conformational search.

Unit-III: QSAR

QSAR: Molecular descriptors, Electronic parameters, Steric parameters, Topological parameters, Quantum-chemical descriptors, Biological parameters, 2D-QSAR, Hansch analysis, Free-Wilson analysis, Topliss analysis and Craig plot, Validation of QSAR models, 3D QSAR models, Success stories of QSAR (Oseltamivir, Saquinavir, Aliskiren, Boceprevir, Norfloxacin, Donepezil), Future scope and applications of QSAR.

Unit-IV: Homology Modeling

Selection of template protein, Alignment of protein sequences, Prediction of protein structures by threading, Protein folding, structure consistency and validation tools, online available homology modeling servers, applications and challenges, homology modeling using Swiss model server and Modeller, homology modeling of human Rhodopsin.

Unit-V: Case studies of drug discovery using Modern drug design tools

Discovery and development of following drugs using various drug design approaches: Captopril, Ranitidine, Monteleukast, Boceprevir, Piragliatin, Saxagliptine, Vorapaxar, Maraviroc, Raloxifene, Sitagliptin, Artemisinin

Reference Books/Articles

Unit-I: (i) Kunal Roy, Supratik Kar and Rudra Narayan Das; Understanding the basics of QSAR for applications in pharmaceutical sciences and risk assessment; ISBN: 978-0-12-801505-6 (2015), Academic press; Elsevier Inc. https://doi.org/10.1016/C2014-0-00286-9 Unit-II: (i) J P Hughes; Principles of early drug discovery; British Journal of Pharmacology; 2011, 162, 1239-1249 (ii) Leonardo G Ferreira; Molecular docking and structure-based drug design strategies; molecules; 2015, 20, 13384-13421; doi:10.3390/molecules200713384 (iii) Dar et al.; Molecular docking: Approaches, types, applications and basic challenges; J Anal Bioanal Tech.; 2017, 8, 2; doi: 10.4172/2155-9872.1000356 (iv) Srinivas Reddy A et al.; Virtual screening in drug discovery-A computational perspective; Current Protein and Peptide Science; 2007, 8, 329-351 Unit-III: (i) Kunal Roy, Supratik Kar and Rudra Narayan Das; Understanding the basics of QSAR for applications in pharmaceutical sciences and risk assessment; ISBN: 978-0-12-801505-6 (2015), Academic press; Elsevier Inc.

https://doi.org/10.1016/C2014-0-00286-9 (ii) Neves B J et al.; QSAR based virtual screening: Advances and applications in drug discovery; Front. Pharmacol; 2018, 9, 1275; doi: 10.3389/fphar.2018.01275 Unit-IV: (i) Muhammed Tilahun Muhammed; Homology modelling in drug discovery: Overview, current applications, and future perspectives; Chem. Biol. Drug Des.; 2019, 93, 12-20; doi: 10.1111/cbdd.1338 (ii) V K Vyas et al.; Homology modelling a fast tool for drug discovery: Current perspectives; Indian Journal of Pharmaceutical Sciences; 2012, 74(1), 1-17; doi: 10.4103/0250-474X.102537 (iii) Andrew Water house et al.; SWISS-MODEL: Homology modelling of protein structures and complexes; Nucleic Acids Research; 2018, 46; Web server issue W296-W303; doi: 10.1093/nar/gky427 (iv) https://salilab.org/modeller/tutorial/basic.html; Modelling lactate dehydrogenase from Trichomonas vaginalis based on a single template, from basic example in Modeller tutorial (v) https://salilab.org/modeller/tutorial/advanced.html; Modelling of a protein-ligand complex based on multiple templates, loop refinement and user specified restraints, from advanced example in Modeller tutorial Unit-V: (i) Case studies in modern drug discovery and development; Edited by Xianhai Huang and Robert G Aslanian; Published 2012 by John Wiley & Sons, Inc. (ii) Accounts in drug discovery: Case studies in medicinal chemistry; Edited by Joel C Barrish, Percy H Carter; Peter T W Cheng and Robert Zahler; 2011; Published by the Royal Society of Chemistry (iii) F George Njoroge, Kevin X Chen, Neng-Yang Shih, John J Piwinski; Challenges in modern drug discovery: A case study of Boceprevir, an HCV protease inhibitor for the treatment of Hepatitis C Virus infection; Accounts of Chemical Research; 2008, 41 (1), 50-59 (iv) Danial Drucker, Chris Easley, Peter Kirk Patrick; Sitagliptin; Nature Reviews in Drug Discovery; 2007, 6, 109-110

IPCH-9.3LAB: NATURAL PRODUCTS LAB (Credits: 2, 6hrs/week)

Extraction of the following compounds from their natural sources, comparison with standards and identification by color reactions

Piperine from pepper
Caffeine from tea leaves
Caffeine from coffee beans
Cineole from eucalyptus leaves
Casein from milk
Lycopene from tomatoes
Menthol from mint leaves
Color reactions of the Natural Products

IPCH-9.4LAB: PEPTIDE CHEMISTRY LAB (Credits: 2, 6hrs/week)

Preparation and identification of Dipeptides and Tripeptides from given amino acids In the process, learn about the purification of peptides, protection & deprotection of various functional groups and coupling reagents

IPCH-9.5LAB: MOLECULAR MODELING AND DRUG DESIGN LAB (Credits: 2, 6hrs/week)

Case studies on applications of computer aided drug design tools:

- 1. Selection of natural products *in silico* for the treatment of Alzheimer's disease
- 2. Quantum chemical calculations and molecular docking of some NSAIDs as 1PGE inhibitors
- 3. PASS based virtual screening for kinase inhibitors
- 4. Ginger components as new leads for the design and development of novel multi-targeted anti-Alzheimer's drugs: A computational investigation
- 5. Molecular docking studies of antimalarial drugs for Malaria
- 6. The integration of pharmacophore-based 3D QSAR modelling and virtual screening in safety profiling: A case study to identify antagonistic activities against adenosine receptor, A2A

Reference Books/Articles:

- 1. Chen et al; A strategy to find novel candidate anti-Alzheimer's disease drugs by constructing interaction networks between drug targets and natural compounds in medical plants; PeerJ; 2018; 6:e4756; DOI 10.7717/peerj.4756
- 2. International Journal of Spectroscopy, Volume 2016, Article ID 5281636, 7 pages http://dx.doi.org/10.1155/2016/5281636
- 3. Pogodin P V et al.; How to achieve better results using PASS-based virtual screening: Case study for Kinase inhibitors; Front. Chem.; 2018, 6, 133; doi: 10.3389/fchem.2018.00133
- 4. Drug Design, Development and Therapy; 2014; 8; 2045-2059
- 5. Prakash N et al.; Molecular docking studies of antimalarial drugs for Malaria; J Comput Sci Syst. Biol.; 2010, 3, 070-073; doi:10.4172/jcsb.1000059
- 6. Fan F et al.; The integration of pharmacophore-based 3D QSAR modelling and virtual screening in safety profiling: A case study to identify antagonistic activities against adenosine receptor, A2A, using 1,897 known drugs; PLoS ONE; 2019, 14(1) e0204378; https://doi.org/10.1371/journal.pone.0204378