BENGALURU CENTRAL UNIVERSITY

M. Sc., Chemistry (CBCS)

Syllabus

(w. e. f. 2019-2020)

VIJAYA COLLEGE R.V. ROAD, BENGALURU-560004

POST GRADUATE DEPARTMENT OF CHEMISTRY

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SYLLABUS 2019-20

1. Name of the Course	:	M.Sc., Chemistry
2. Duration of the Course	:	Two Years (FOUR SEMESTERS, CBCS)
3. Eligibility	:	A candidate must have secured 40% marks
		in the aggregate and studied Chemistry
		(cognate subject) securing 50 % marks in this
		subject at the B Sc., level and studied
		Mathematics at $10 + 2$ or Pre-university
		level.
		40 + Supernumerary seats + Payment
4. Intake	:	seats= 60 (Total)
5. Admission	:	As per University regulations

Scheme of Study and Examination M. Sc., CHEMISTRY

			I Semes	ter				
Code No.	Title	Theory/ Practical (Hrs/ Week)	Total No.of Hrs/ Semester	Duration of Exam. Hours	Max. Marks (Exam)	Continuous Evaluation	Total Marks	Credits
Ch-101	Inorganic Chemistry I	4	52	3	70	30	100	4
Ch-102	Organic Chemistry I	4	52	3	70	30	100	4
Ch-103	Physical Chemistry I	4	52	3	70	30	100	4
Ch-104	Analytical Chemistry	4	52	3	70	30	100	4
Ch-105	Mathematics for Chemists (Soft Core)	3	36	3	70	30	100	2
Ch-106	Practical-I Inorg/Org/Phy	4	60	4	35	15	50	2
Ch-107	Practical-II Inorg/Org/Phy	4	60	4	35	15	50	2
Ch-108	Practical-III Inorg/Org/Phy	4	60	4	35	15	50	2
Ch-109	Practical-IV Inorg/Org/Phy Total	4	60	4	35	15	50 700	2 26
	marks/credits						700	20

				II Semeste	er			
Code No.	Title	Theory/ Practical (Hrs/ Week)	Total No.of Hrs/ Semester	Duration of Exam. Hours	Max. Marks (Exam)	Continuous Evaluation	Total Marks	Credits
Ch-201	Inorganic Chemistry-II	4	52	3	70	30	100	4
Ch-202	Organic Chemistry-II	4	52	3	70	30	100	4
Ch-203	Physical Chemistry-II	4	52	3	70	30	100	4
Ch-204	Spectroscopy-I	4	52	3	70	30	100	4
Ch-205	Green Synthesis / Photo Chemistry (Soft Core)	3	36	3	70	30	100	2
Ch-206	Practical-I Inorg/Org/Phy	4	60	4	35	15	50	2
Ch-207	Practical-II Inorg/Org/Phy	4	60	4	35	15	50	2
Ch-208	Practical-III Inorg/Org/Phy	4	60	4	35	15	50	2
Ch-209	Practical-IV Inorg/Org/Phy Total marks/credits	4	60	4	35	15	50 700	2 26

				III Semest	ter			
Code No.	Title	Theory/ Practical (Hrs/	Total No.of Hrs/	Duration of Exam.	Max. Marks (Exam)	Continuous Evaluation	Total Marks	Credits
		Week)	Semester	Hours	()			
	Organic Reaction Mechanisms	4	52	3	70	30	100	4
Ch-302	Chemistry of Natural Products	4	52	3	70	30	100	4
	Organic Spectroscopy				70	30		
Ch-303		4	52	3	10	50	100	4
Ch-304	Open Elective	4	52	3	70	30	100	4
Ch-305	Practical-I Organic Chemistry	4	60	4	35	15	50	2
Ch-306	Practical-II Organic Chemistry	4	60	4	35	15	50	2
Ch-307	Practical-III Organic Chemistry	4	60	4	35	15	50	2
Ch-308	Practical-IV Organic Chemistry	4	60	4	35	15	50	2
	Total marks/credits						700	26

	IV Semester							
Code No.	Title	Theory/ Practical	Total No.of	Duration of	Max. Marks	Continuous Evaluation	Total Marks	Credits
		(Hrs/ Week)	Hrs/ Semester	Exam. Hours	(Exam)			
Ch-401	Organometallic and Heterocyclic Chemistry	4	52	3	70	30	100	4
	Stereochemistry & Retrosynthetic							4
Ch-402	Analysis	4	52	3	70	30	100	
Ch-403	Organic Synthesis	4	52	3	70	30	100	4
Ch-404	Medicinal Organic Chemistry	4	52	3	70	30	100	4
Ch-405	Practical-V Organic Chemistry	4	60	4	35	15	50	2
Ch-406	Practical-VI Organic Chemistry	4	60	4	35	15	50	2
Ch-407	Practical-VII Organic Chemistry	4	60	4	35	15	50	2
Ch-408	Practical-VIII Organic Chemistry	4	60	4	35	15	50	2
	Total marks/credits						700	26

Practical: 30 marks for experiment + 5 marks for Viva-Voce IA : Marks based on Test + Assignment + Seminar + Records

Scheme for continuous evaluation Theory (each paper)						
Tests*	s* : 20 marks					
Total	1 : 20 Marks					
*	Two tests will be conducted and the average marks of the two tests will be taken for Continuous assessment.					
*	There should be minimum marks of 8 to be scored out of 20 for getting eligibility to attend the final University examination.					

Practicals: (each practical)

Test (1 Test)	15 marks	
Total	15 marks	

QUESTION PAPER PATTERN

Semester I/II	Sub: Chemistry	
Time: 3 Hrs		Max. Marks: 70
Note: Answer question Number one	and any SIX in the remaining.	
1. Answer any TEN sub divisions fr	rom the following	(10x2=20)
a) b) c) d) e) f) g) n) i) ;)) k) l)		
2 to 8		(5x10=50)
2.		
a) b) c)		(5+5) or (6+4) or(4+3+3)

SEMESTER – I

Ch-101 INORGANIC CHEMISTRY- I

UNIT- I

Chemical Bonding- VSEPR model, shapes of molecules-ClF₃, ICl₄, TeF₅, I₃, TeCl₆²⁻, XeF₆, SbCl₆³⁻, IF₇, ReF₇, XeF₈²⁻, TaF₈³⁻; Bent rules and energetics of hybridization; electronegativity-Pauling, Allred-Rochow and Mulliken, electronegativity and partial ionic character; Bonds- Multicenter, Synergic and Agostic bonding. Lattice energy: Born-Lande equation, Kapustinskii equation; Fajan's rules- polarizability and partial covalent character, radius-ratio rules-limiting radius ratios of trigonal, tetrahedral, octahedral and cubic. Structures of solids-NaCl, CsCl, ZnS(zinc blende and wurtzite), rutile(TiO₂), pervoskite(CaTiO₃), fluorite and anti fluorite. Zintl ions, Molecular orbital theory: formation of sigma, pi and delta bonds, LCAO and MO diagrams of heteronuclear diatomic (CO, NO, HF and ICl) and triatomic molecules (CO₂ and NO₂⁻).

UNIT-II

13h

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Chemistry of main group elements:- Boranes- nomenclature, synthesis, structure and bonding in boranes, styx code, carboranes- classification, structures of ortho, meta, para- $C_2B_{10}H_{12}$, Wades rules, Metallocarboranes- synthesis and structure of $[Fe(\eta^5-C_2B_9H_{11})_2]^2$, $Fe(\eta^5-C_2B_9H_{11})(\eta^5-C_5H_5)$, $[Mo(CO)_3(\eta^5-C_2B_9H_{11})]^2$, synthesis, structure and bonding in borazine, phosphazenes- synthesis, structure and bonding in (PNCl₂)₃, S,N- compounds-S₄N₄, S₂N₂ and polythiazyl.

Silicates:- Principles of silicates structures, classification with examples-ortho, pyro, cyclo, ino, phyllo and tecto silicates, isomorphous replacement; zeolites- sodalite and pentasil units, synthesis and structures of ZSM-5, zeolite A, faujasite and their uses.

UNIT-III

13h

HSAB concept: Basis of HSAB concept, acid-base strength, hardness and softness, symbiosis,

applications and limitations of HSAB concept; Acid- base concept in non-aqueous media, reactions in BrF3, N2O4, anhydrous H2SO4, CH3CO₂H. Isopoly and heteropoly acids of W and Mo, preparations, properties, structure and applications.

Stereoisomerism:- Chirality, optical activity- CD, ORD, Cotton effect, absolute configuration of

metal complexes, magnetic circular dichroism and its uses.

UNIT-IV

13h

Metal clusters- factors favouring M-M bond, classification, synthesis, structure and bonding

in $[Re_2Cl_8]^{2-}$. Metal carbonyl clusters- LNCC's and HNCC's. Electron counting in carbonyl clusters, Wades-Mingos and Lauher rules.

Nuclear Chemistry-The atomic nucleus-elementary particles, quarks, classification of nuclides based on Z and N values, nuclear stability, nuclear potential, binding energy. Nuclear

Models: Shell model-salient features, forms of the nuclear potential, filling of orbitals, nuclear

configuration, Liquid drop model. Radioactivity, radioactive decay kinetics, Parent-daughter decay-growth relationship-secular and transient equilibria, theories of α , β^- , β^+ and γ -decay, internal conversion, Auger effect.

SUGGESTED BOOKS

- 1. Basic Inorganic Chemistry- F. A. Cotton, G. Wilkinson and P. L. Gaus; John Wiley and sons. Inc, 3rd edition (2004).
- 2. Advanced Inorganic Chemistry, F. A. Cotton and G. Wilkinson. 6th edition (1999).
- 3. Inorganic Chemistry, J. E. Huheey, E. A. Keiter and R. L. Keiter, IV edition Addison; Wesley (1993).
- 4. Inorganic Chemistry, D. F. Shriver, P. W. Atkins and C. H. Langford, V edition ELBS; Oxford University Press, (2010)
- 5. Chemistry of elements; N. N. Greenwood and A. E. Earnshaw, Butterworth, II edition Heinemann (1997).
- 6. Concise Inorganic Chemistry, J. D. Lee, 5th edition; (1996).
- 7. Essentials of nuclear chemistry, H. J. Arniker, 4th edition; NAIL publishers (2011) Chapters 1, 3 and 4.
- Nuclear and Radio chemistry; G.Friedlander, J.W.Kennedy, ES Macias and JM Miller; 1981, Chapters 8and 9.
- 9. Inorganic Chemistry, Gary. L. Miessler and Donald . A. Tarr 5th Edition; (2014).
- 10. Inorganic Chemistry CE House croft and A G Sharpe 4th edition, pearson (2012).

Ch-102: ORGANIC CHEMISTRY- I

UNIT-I

Nature of Bonding in Organic Molecules

13h

Delocalized chemical bonding: Conjugation, cross conjugation, resonance. Hyperconjugation. Tautomerism.

Aromaticity: Huckel's MO theory. HMO diagram for benzene. Huckel's rules of aromaticity. Aromatic systems with electron numbers other than six (including azulene, tropone, tropolone and annulenes). Anti-aromaticity. Aromaticity in benzenoids. Homo-aromaticity. Alternant and non-alternant hydrocarbons. Energy levels in odd and even-alternant hydrocarbons, energy levels for the benzyl cation, benzyl free-radical and benzyl carbanion.

Mesoionic compounds. Heteroannulenes. Fullerenes: C-60.

<u>Synthetic Molecular Receptors:</u> Definition and significance. Structure and function of receptors with molecular clefts, molecular tweezers, receptors with multiple hydrogen bonding sites. Crown ethers, cryptates, cyclodextrins, cyclophanes, catenanes and rotoxanes, calixarenes, ionophores and micelles.

UNIT-II

Reaction Mechanisms: 13h

<u>Reactive intermediates:</u> Generation, structure, stability and reactivity of carbocations, carbanions, carbon free radicals, carbenes. Non-classical carbocations, nitrenes.

Reactions and mechanisms: Thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammond postulate, Curtin-Hammett principle. Potential energy diagrams, transition states and intermediates.

Methods of determining mechanisms: Based on the structure of products, determination of the presence of intermediates, isotopic labeling, isotope effects, from stereochemical evidence.

Acids and bases: Hard and soft acids and bases. Effect of structure on the strengths of acids and bases.

Effect of structure on reactivity: Resonance and field effects; steric effects. The Hammett equation and linear free energy relationship, substituent and reaction constants. Taft equation.

Aliphatic substitution reactions:

Nucleophilic substitution reaction at a saturated carbon: SN1, SN2, and SET mechanisms. Effect of substrate structure, attacking nucleophile and leaving group. Neighbouring group participation by sigma and pi bonds. Anchimeric effect. Ambident nucleophiles and substrates.

Electrophilic substitution reaction at a saturated carbon:_SE1, SE2, and SEi mechanisms. Effect of substrate structure, leaving group and solvent polarity on the reactivity.

<u>UNIT-III</u>

Stereochemistry

Projection formulae: Fischer, Newman, Sawhorse and flying wedge projections - their interconversions for acyclic and cyclic compounds.

*Conformational analysis:*_D/L, R/S and M/P conventions. Cahn-Ingold Prelog (CIP) sequence rules.

Optical isomerism: Elements of symmetry and chirality. Chirality in compounds with a stereogenic centre. Center of chirality, axis of chirality, plane of chirality and helicity. Stereochemistry of allenes, alkylidene cycloalkanes and spiranes (with a stereogenic axis), biphenyls, cyclophanes, ansa compounds, *trans*-cyclooctene, helicenes, benzphenanthrenes. Configurational nomenclature. *Conformational analysis*: Conformational analysis of cycloalkanes: cyclobutane, cyclopentane, cyclohexanes (mono-substituted e.g., methyl, *iso*-propyl, *tert*-butyl and di-substituted cyclohexanes e.g., dialkyl-, dihalo-, diols), and cycloheptane. Nomenclature and conformations of fused rings and bridged ring systems. *Prochirality*: Enantiotopic and diastereotopic atoms, groups and faces. [Si/Re]. Basics of Cram's and Prelog's rules of asymmetric induction.

UNIT-IV

Carbohydrates:

Introduction. Determination of configuration of the mono saccharides, conformational analysis of monosaccharides. Synthesis of aldonic, uronic, aldaric acids and alditols Derivatives of monosaccharides: acetals, ethers,

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aminosugars and deoxysugars. Structural elucidation of sucrose and maltose. Structures of lactose, gentiobiose and meliobiose. Photosynthesis of carbohydrates.

Heterocyclic compounds:

Introduction. Nomenclature of simple and fused heterocyclic compounds: Hantzsch-Widman method. Synthesis and reactions of pyrazole, imidazole, oxazole, isoxazole, thiazole, isothiazole. Synthesis of indole, benzimidazole, benzoxazole and benzisoxazole and coumarins.

SUGGESTED BOOKS

1. Organic Chemistry, R T Morrison, R N Boyd and S K Bhattacharjee, 7th edition,

Pearson, (2018).

2. Organic Chemistry, J Clayden, N Greeves and S Warren, 2nd edition, Oxford

University Press, (2014)

3. Advanced Organic Chemistry – Reactions, Mechanism and Structure, J March,

John Wiley (2008).

Advanced Organic Chemistry, F A Carey and R J Sundberg Plenum, (2000).

5. A Guide Book to Mechanism in Organic Chemistry, P Sykes, 6th edition, Pearson, (2003).

6. Structure and mechanism of Organic Chemistry, C K Ingold, 2nd Edition, CBS,

(2016).

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7. Principles of Organic Synthesis, 3rd edition, R O C Norman and J M Coxon,

Blackie Academic and Professional (Indian Reprint), (2012).

Stereochemistry, V R Dani, Asian Books, New Delhi, (2014).

9. Stereochemistry of Organic Compounds, D Nasipuri, 3rd edition, New-Age International,

(2018).

10. Organic Stereochemistry, M J T Robinson, Oxford University Press, (2005).

11. Stereochemistry of Carbon Compounds, E L Eliel, S H Wilen and L N Mander.

John Wiley, (1994).

12. Stereochemistry at a Glance J Eames, J M Peach, Blackwell, Oxford,

(2003).

13. Heterocyclic Chemistry at a Glance, II edition, J A Joule and K Mills, Wiley, New York,

(2012).

14. Organic Chemistry, Volume I, I L Finar, 6th edition, Pearson, (2018).

15. Organic Chemistry, Volume II, I L Finar, 6th edition, Pearson, (2018

Ch-103 PHYSICAL CHEMISTRY- I

UNIT-I

Quantum Mechanics-I

Introduction to quantum mechanics. Schrödinger wave equation. Time-independent and time dependent Schrödinger wave equations and the relation between their solutions. Eigen functions and Eigenvalues. Physical Interpretation of wave function. Concepts of Operators: Laplacian, Hamiltonian, Linear and Hermitian operators. Angular Momentum operators and their properties. Commutation of operators. Normalization, orthogonality and orthonormality of wave functions. Average (expectation) values. Postulates of quantum mechanics. Solutions of Schrödinger wave equation for a free particle, particle in a ring, particle in a three dimensional box. Quantum mechanical degeneracy, tunneling (no derivation). Application of Schrödinger equation to harmonic oscillator, rigid rotator. Eigen functions and eigenvalues of angular momentum. Ladder operator method for angular momentum.

UNIT-II

Quantum Mechanics-II

Schrödinger equation to hydrogen atom in spherical polar co-ordinates. Solution of equation and statements of solution of R equation. Total wave functions of hydrogen atom. Quantum numbers and their characteristics. List of wave functions for few initial states of hydrogen like atoms. Diagrams of radial and angular wave functions. Radial and angular distribution function and their significance. Electron spin

(Stern-Gerlach experiment), spinorbital, anti symmetry and Pauli-exclusion principle, Slater determinants. Coupling of Angular momenta. Russell-Saunders and JJ-coupling, Atomic Term symbols. Spin-orbital interaction and explanation of term multiplicities (Na-D doublet). Zeeman effect.

Approximate methods: Need for approximate methods. Perturbation method. Rayleigh Schrödinger perturbation theory for time-independent non-degenerate system. Application to electron in a box under the influence of an electric field. Application to He atom. Variation theory-statement and proof. Application of variation method to particle in a one-dimensional box and He atom.

UNIT-III

Chemical Dynamics-I

Macroscopic and microscopic kinetics, Review of theories of reaction rate-Collision theory and

Transition state theory, Comparison of collision theory with transition state theory, Arrhenius

equation- characteristics, Significance of energy of activation, Temperature coefficient and its

evaluation. Thermodynamical formulation of reaction rates (Wyne-jones and Eyring treatment),

Reaction between ions in solutions – Influence of ionic strength on reaction rates (primary and

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secondary salt effects).

Concept of Steady state kinetics, Chain reactions – chain length and chain inhibition, comparison

of photochemical and thermal reactions, Mechanisms of thermal and photochemical reactions

between hydrogen-bromine and hydrogen-chlorine. Comparative study of thermal and

photochemical hydrogen-halogen reactions. Pyrolysis of acetaldehyde, Decomposition of ethane.

Kinetics of fast reactions- Introduction, Study of reactions by relaxation method (Temperature

and pressure jump), flow method (Plug flow method and Stopped flow method), Flash photolysis

and Shock tube method.

UNIT-IV

Chemical Dynamics-II

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Kinetics of homogeneous catalysis: kinetics of auto catalytic reactions, kinetics of acid-base catalysed reactions. Comparison of enzyme catalysed and chemical catalysed reactions, Mechanism (Lock and Key theory), Kinetics of enzyme catalyzed reactions – Henri-MichaelisMenten mechanism, Significance of Michaelis-Menten constant, Lineweaver-Burk plot. Effects of enzyme concentration, pH, Temperature, Activators and Inhibitors on enzyme activity.

Unimoleuclar reactions: Perrin theory, Lindemann theory, and Hinshelwood theory.

Surface chemistry: Types of adsorption isotherms, Effect of temperature on adsorption, Mechanical adsorption, Estimation of surface area using BET equation, Gibbs adsorption isotherm and its significance, Surface tension and surface energy, Pressure difference across curved surface (Laplace equation), Vapour pressure of droplets (Kelvin equation), Surface film on liquids (electro-kinetic phenomena), Catalytic activity of surfaces.

SUGGGESTED BOOKS

- 1. Physical Chemistry- P. Atkins and J. D. Paula, 9th Edn., Oxford University Press (2010).
- 2. Physical Chemistry: A Molecular Approach, D. A.McQuarie and Simon, Viva, New Delhi, (2003).
- 3. Introduction to Quantum Chemistry, A. K. Chandra, 3rdEdn. Tata McGraw Hill, (1991).
- 4. Quantum Chemistry, Ira. N. Levine, Prentice Hall, New Jersey, (1991).
- 5. Quantum Chemistry, R. K. Prasad, New Age International, 4thEdn., (2010).
- 6. Quantum Mechanics by G R Chatwal and S K Anand, Himalaya Publications, 8thEdn, 2012.
- 7. Chemical Kinetics- K. J. Laidler, McGraw Hill. Inc. New York (1988).

- 8. Principles of Chemical Kinetics House J. E. Wm C Brown Publisher, Boston, (1997).
- 9. Kinetics and Mechanism of Chemical Transformations- J. Rajaraman and J. Kuriakose, Mc Millan India Ltd. (2011).
- 10. Biochemistry, Geoffrey Zubay, 2nd Edn., Macmillan Publishing Co. New York (1988).
- 11. Physical Chemistry of Surfaces- A. W. Adamson, Wiley-Interscience Publisher Inc., New York (1997).
- 12. Introduction to surface chemistry and Catalysis by Gabor A. Somorjai<u>and</u> Yimin Li, John 2ndEdn. Wiley and Sons Ltd, Hoboken, United States, 2010.

Ch-104 Analytical Chemistry

UNIT – I Basic concepts

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Safety measures in chemical laboratories, Fire hazards, toxic chemicals: Acids/bases/solvents handling, storage, dilution, disposal of chemicals, acid/ solvent bottles etc. toxic chemicals sampling and handling hazards, safety data sheets, miniaturization of analytical instruments, their significance in modern chemical analysis.

Preparation of dilute acids from concentrated/fuming acids like H₂SO₄, handling liquid bromine, elemental mercury, solvent ether, liquor ammonia, liquid nitrogen.

Errors in chemical analysis: absolute, relative error, random error distribution, Gaussian curve, Limitations of analytical methods, determinate and indeterminate errors, minimization of errors. Accuracy and precision, distribution of random errors, the normal error curve. Statistical treatment of finite samples - measures of central tendency and variability: mean, median, range, standard deviation, variance, confidence limits, Comparison of an experimental mean and a true mean. F-test, rejection of result - Q-test, Student's t-test, numerical problems.

UNIT-II Quantitative Analysis-Classical methods

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Classification of analytical methods, types of instrumental analysis, factors influencing choice of analytical method, qualitative and quantitative analysis, Units used in chemical analysis, their conversion, ppm, ppb, ppt etc.

Titrimetry

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Acid-Base: Theory of indicators, Ex: Phenophthalien, Methyl red. Titration curves for mono functional acid and base, pH calculations, fractions of phosphoric acid species as a function of pH. Titration curves for H_3PO_4 .

Complexometry: Theory of metal ion indicators, EDTA titrations, suitability of polydentate ligands as titrants, expressions for the different forms of EDTA in solution as a function of pH, conditional stability constants, effect of pH and nature of titration curve. Masking and demasking, type of EDTA titrations, titrations involving monodentate, bidentate and polydentate ligands.

Redox: Mechanism of indicator action, criteria for the selection of indicators. Feasibility of redox titration. Titration of multicomponet system. Nernst equation. Applications: Oxidants such as Ce(IV), bromate, Iodates.

Precipitation: Solubility product. Theoretical principles of precipitation: Titration curve, end point detection, Mohr, Volhard and adsorption indicators. Applications: Estimation of F^- , K^+ , $CO_3^{2^-}$, $C_2O_4^{2^-}$, acetylenes and mixture of halides.

Gravimetry

Quantitative precipitation, *Precipitation from Homogeneous Solution (PFHS)*, Formation and treatment of precipitates, co-precipitation, post precipitation. Conditions for precipitation, washing, drying and igniting the precipitates, Important precipitating agents such as DMG, oxine, thiocyanate and their significance in inorganic analysis. errors in gravimetric analysis.

Unit-III - Quantitative Analysis - Instrumental methods

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Electromagnetic radiation, interaction with matter, absorption, Beer-Lambert's law, derivation, molar absorptivity, Sandell sensitivity, Ringbom plot, deviations, limitations, Calibration with standards, standard addition, internal standard addition, limit of detection, limit of quantification, Instrumentation, radiation sources, wavelength selection devices, optical slits, single beam and double beam instruments, photo electric colorimeter, scanning devices, merits and limitations, numerical problems on application of Beer's law.

Unit IV- Separation Methods

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Solvent Extraction – Types, batch, continuous, efficiency, selectivity. Distribution coefficient, Nernst distribution law, derivation, factors affecting the partition, applications. Chromatography – Types, Terminology, Principles of paper, thin layer, column, gas chromatography, column efficiency, plate theory, factors affecting the column efficiency, band broadening, R_f factor, Van-Deemter equation, medium performance liquid

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chromatography, high performance liquid chromatography, reserved phase liquid chromatography, super critical fluid chromatography, characteristics of super critical fluids, 2D-thin layer chromatography, electrophoresis, principles, applications etc. numerical problems on solvent extraction, Rf factor and van Demeter equation.

Suggested books:

- 1. Fundamental of Analytical Chemistry, D.A. Skoog, D.M. West, Holler and Crouch, 8th edition, Saunders College Publishing, New York, 2005.
- 2. Analytical Chemistry, G.D. Christian, 6th edition, John Wiley & Sons, Inc, India, 2004.
- 3. Quantitative Analysis, R.A. Day and A.L. Underwood, 6th edition, Prentice Hall, Inc. New Delhi, 1993
- 4. Vogel's Textbook of Quantitative Chemical Analysis, J. Mendham, R.C. Denney, J.D. Barnes and M.J.K. Thomas, 6th edition, Third Indian Reprint, Pearson Education Pvt. Ltd., New Delhi, 2003.
- 5. Analytical Chemistry Principles, John H. Kennedy, 2nd edition, Saunders College Publishing, California, 1990.
- 6. Principles and Practice of Analytical Chemistry, F.W. Fifield and Kealey, 3rd edition, Blackwell Sci., Ltd. Malden, USA, 2000.
- 7. Modern Analytical Chemistry, David Harvey, McGraw Hill, New Delhi, 2000.
- 8. Practical Volumetric Analysis, Peter A C McPherson, RSC, Cambridge, UK, 2015.
- 9. Analytical Chemistry for Technicians, John Kenkel, 4th edn. CRC Press, London, 2014.
- 10. Undergraduate Instrumental Analysis, J.W. Robinson, E.M. Skelly Frame, G. M. Frame II, 6th edn. Marcel Dekker, New York, 2009.

Ch-105 MATHEMATICS FOR CHEMISTS

UNIT-I

1 2 h

Vectors: vectors, dot and cross products; scalar and vector triple products and their applications.

Tensors and their applications.

Matrix Algebra: Review of different types of matrices (including Hermetian and skew Hermetian); matrix addition and multiplication; determinant of a square matrix, transpose, adjoint and inverse of a square matrix. Solution to system of linear equation (a) by matrix method and (b) by Cramer's Rule. Characteristic equation of a square matrix, eigenvalues

and eigenvectors.

UNIT-II

1 2 h

1 2 h

Calculus: Rule for differentiation; Chain rule (for $f(x)=U^n$, sin u, log u etc). Implicit

differentiation and parametric differentiation and successive differentiation of order 2 (for

explicit functions only).

Applications of differentiation:

Derivative as a slope of the tangent, derivative as a rate measure-velocity and acceleration. Increasing and decreasing functions-Maxima and minima-second derivative test-point of inflections-problems restricted to polynomial.

UNIT-III

Integrations: Basic rules-simple substitution-Method of partial fractions-Integration by parts.

Define integral and application to areas of plane curves.

Functions of several variables: partial derivatives; co-ordinate transformation from cartesian co-ordinates to spherical and cylindrical coordinates and vice-versa.

Elementary differential equation: Variable separable, exact first order equations, linear and homogeneous equation.

Second order homogeneous differential equation with constant coefficients f(D), y=0. Solution

of differential equation by power series method.

Fourier series: Simple problems.

Probability: Review of permutations and combinations. Probability and addition theorem for mutually exclusive events and multiplication theorem for independent events. Curve fitting-Method of least squares.

SUGGESTED BOOKS

- 1. Mathematical Preparation for physical chemistry, F. Daniells, M.Graw Hill Inc., US, 1959
- 2. Mathematics for chemists, D. M. Hirst, Chemical Publishing Company Incorporated, New York, 1979.
- 3. Mathematics for chemists, P. G. Francis, Springer, 2011.
- Basic Mathematics for chemists, P. Tebutt, Wiley-Blackwell, 1994.
 Calculus and analytic geometry, 9th edition, G. B. Thomas, R.L. Finney, Addison-Wesley Publishing Company, Inc. 1996.
- 6. Short Course in differential equations, Rainvilles and Bedient, IBH publishers, 1968.

7. Mathematics for chemistry, G. Doggett and B. T. Sutcliffe Longmann Publishers, 1995.

INORGANIC CHEMISTRY PRACTICALS (4 days a week, 4 hours a day)

C-106 Inorganic Chemistry Practical-I

Semi micro qualitative analysis of mixtures containing two anions, two common cations and one less familiar elements: W, Mo, Ce, Zr, V and Li.

C-107 Inorganic chemistry practical-II

Preparation of inorganic complexes:

- 1. Cis- potassium dioxalatodiaquachromium(III) complex.
- 2. Hexamminecobalt(III) chloride.
- 3. Mercury tetrathiocyanatocobaltate.
- 4. Pentamminechlorocobalt(III) chloride.
- 5. Potassium tris(oxalato)ferrate trihydrate.
- 6. Potassium tris(oxalato)aluminate trihydrate.

PHYSICAL CHEMISTRY PRACTICALS (4 days a week, 4 hours a day)

C-108 Physical Chemistry Practical -I

1. Study of Acid catalysed hydrolysis of methyl acetate at lab temperature and reporting the calculated

and graphical rate constants

2. Determination of Velocity constant for the saponification of Ethyl acetate at lab temperature and

comparing it with graphical value.

3. Verification of Beer's Law: Colorimetric estimation of Cu^{2+} ions and reporting the Molar extinction

coefficient.

4. Determination of heat of solution of a sparingly soluble salt.

5. Colorimetric estimation of Fe^{2+} ions in a given solution by titrating FAS versus KMnO₄ solution.

6. Study of kinetics of the reaction between KI ad K₂S₂O₈solution.

7. Construction of phase diagram of two component systems and determination of Ec , ET and the

Composition of given unknown.

- 8. Determination of partial molar volume of solute water system by apparent molar volume method.
- 9. Analysis of a binary mixture by viscosity measurement method.

10. Verification of Freundlich and Langmuir isotherm for adsorption of oxalic/acetic acid on activated charcoal.

C-109 Physical Chemistry Practical -II

Conductometric Experiments

1. Precipitation titration of lithium sulphate versus $BaCl_2$ and reporting the concentration of Li_2SO_4 .

- 2. Determination of concentration of a weak acid by titrating against a weak base.
- 3. Determination of a dissociation constant of weak acid (CH3COOH).
- 4. Determination of Equivalent conductance of a given strong electrolyte.

5. Determination of the concentration of a strong acid and a salt in a given a mixture of by titrating

against a strong base.

Potentiometric Experiments

- 6. Determination of single electrode potential of Cu²⁺/Cu and estimate the given unknown concentration.
- 7. Determination of single electrode potential of Zn²⁺/Zn and estimate the given unknown concentration.
- 8. Titration of AgNO₃ versus KCl and estimation of the concentration of AgNO₃.

9. Determination of pKa and Ka values of the weak acid by titrating against a strong base using

quinhydrone electrode.

10. Determination and comparison of pH values of buffer solutions by using quinhydrone electrode

and glass electrode.

SUGGETED BOOKS

1. Advanced Practical Physical Chemistry by J. B. Yadav, GoelPublications, Meerut (2012).

2. Senior Practical Physical Chemistry by B. C. Kosla, Simla Printers, New Delhi (1987).

3. Experimental Physical Chemistry by Daniel et al., McGraw Hill, New York (1962).

4. Practical Physical Chemistry by A.M James and P. E. Pritchard, Longman's Group Ltd (1968).

5. Experimental Physical Chemistry by Wilson, Newcombe& others, Pergamon Press, New York

(1962).

6. Experimental Physical Chemistry by R. C. Behra and B Behra, Tata McGraw, New Delhi (1983).

7. Experimental Physical Chemistry by V. D. Atavale and ParulMathur, New Age International,

New York (2001).

8. Practical's in physical chemistry A. Modern Approach by P.S Sindhu, Mac. Millan Publishers,

Delhi (2006).

II SEMESTER

Ch-201: INORGANIC CHEMISTRY- II

UNIT-I

13h

Metal-Ligand equilibria in solution- Step-wise and overall formation constant and their relationship, trends in step-wise constant, kinetic and thermodynamic stability of metal complexes, factors affecting the stability of metal complexes with reference to the nature of the metal ion and ligand, chelate effect, macrocyclic effect and their thermodynamic origin. Determination of binary formation constant by pH metry, spectrophotometry, polarography and ion exchange methods.

Structure and bonding- hydride, dihydrogen, dioxygen, isocyanide, N2 and tertiary phosphine complexes of transition metals, metal carbonyls-terminal and bridge carbonyls, detection, metal nitrosyls- terminal (linear and bent) and bridge.

UNIT-II

13h

Metal- ligand bonding- Coordination numbers 3 to 8. Crystal field theory, salient features, spectrochemical series, splitting of d-orbitals in tetrahedral, square planar, trigonal bipyramidal, square-pyramidal and octahedral geometry, applications of CFT- colors of

transition metal complexes, magnetic properties of octahedral complex, Jahn Teller distortion, CFSE and their uses, factors affecting CFSE, limitations of CFT, experimental evidences for metal-ligand covalent bonding in complexes, nephelauxetic effect, Ligand Field Theory, MO theory: tetrahedral and octahedral complexes (including π -bonding), angular overlap model. Stereochemical non-rigidity and its detection.

UNIT-III

13h

Electronic spectra of coordination compounds- Spectroscopic ground states, selection rules, term symbols for d^a ions, Racah parameters, Orgel, Correlation and Tanaube-Sugano diagrams, spectra of 3d metal-aqua complexes of trivalent V, Cr, divalent Mn, Co and Ni, CoCl4², calculation of Dq, B and β parameters, CT spectra. Spectral properties of Lanthanide and Actinide metal complexes.

UNIT-IV

13h

Magnetic properties of coordination compounds- Types of magnetism, temperature effect, magnetic susceptibility and its determination- Gouy, Faraday, VSM method. Diamagnetic correction, orbital contribution, spin-orbital coupling, ferro- and antiferromagnetic coupling, spincrossover. Magnetic properties of Lanthanide and Actinide metal complexes.

Photochemical reactions of transition metal complexes: Basic photochemical processes, Kasha's rule, quantum yield, Jabolnskii diagrams, photo substitution reactions, photo-redox reactions, ligand photoreactions.

SUGGESTED BOOKS

1. Advanced Inorganic Chemistry- F. A. Cotton, G. Wilkinson and P. L. Gaus; John Wiley and sons. Inc, 6th edition (1999).

2. Chemistry of elements- N. N. Greenwood and A. E. Earnshaw, 2nd edition, Butterworth Heinemann (1997).

3. Inorganic Chemistry J. E. Huheey, E. A. Keiter and R. L. Keiter, 4th edition; Addison; Wesley (1993).

4. Inorganic Chemistry, D. F. Shriver, P. W. Atkins and C. H. Langford, 5th edition, ELBS; Oxford University Press, (2010

5. Inorganic Electronic spectroscopy, A. B. P. Lever, 2nd edition, Elsevier. (1984).

6. Magnetochemistry, R.L. Carlin, Springer Verlag (1986).

7. Electronic Absorption Spectroscopy and related Techniques, D. N. Sathyanarayana, University Press (2001).

8. Inorganic Chemistry A Unified Approach by W. W. Porterfield, Elsevier 2005 2nd edition.

9. Inorganic chemistry G L Miessler, P J Fisher and D A Tarr 5th edition (2008).

Ch-202 ORGANIC CHEMISTRY – II

UNIT-I

Aromatic Substitution Reactions

<u>Electrophilic Substitution Reactions</u>: The arenium ion mechanism. Orientation and reactivity. Energy profile diagrams. The *ortho/para* ratio, *ipso* attack, orientation in other ring systems.Quantitative treatment of reactivity in substrates and electrophiles. Effect of leaving group. Amination, sulfonylation reactions; Diazonium coupling, Vilsmeier-Haack reaction, Gatterman reaction, Gatterman-Koch reaction and Hoesch reaction.

<u>Nucleophilic substitution reactions</u>: The SNAr, SN1, benzyne and SRN1 mechanisms. Reactivity: effect of substrate structure, leaving group and attacking nucleophile. Goldberg reaction, Bucherer reaction, Schiemann reaction, von Richter reaction, Sommelet-Hauser and Smiles rearrangements.

UNIT-II

Addition Reactions

<u>Addition to carbon-carbon multiple bonds</u>: mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals. Regio-, stereo- and chemo- selectivities. Orientation and reactivity. Addition to cyclopropane ring. Hydrogenation of double and triple bonds, hydrogenation of aromatic rings. Addition of alkenes and/or alkynes to alkenes and/or alkynes. Ene synthesis. Michael reaction.

<u>Addition to carbon-heteroatom multiple bonds</u>: Mechanism of metal hydride reduction (NaH, LiH, LiAlH₄, NaBH₄) of saturated and unsaturated carbonyl compounds, acids, esters and nitriles. Addition of Grignard reagents and organolithium reagents to carbonyl compounds and unsaturated carbonyl compounds. Conversion of aldehydes to nitriles. Hydrolysis of nitriles and addition of amines to isocyanates. Formation of xanthates. Wittig, Mannich and Stobbe reactions.

UNIT-III

Elimination Reactions

The E2, E1 and E1cB mechanisms and their spectrum.E2C and E2H mechanisms. Orientation of the double bond.Reactivity-effects of substrate structure, attacking base, the leaving group and the medium. Mechanism and orientation in pyrolytic 13h

13h

elimination reactions (including Chugaev reaction).

Rearrangement Reactions:

<u>*Carbon-carbon*</u>: Wagner-Meerwein, Pinacol-Pinacolone, Fries, Benzil-benzilic acid rearrangements, Wolff rearrangement and Arndt-Eistert reaction, Tiffeneau-Demjanov reaction, Fritsch-Buttenberg-Wiechell rearrangement. Favorskii rearrangement, Dienone-phenol rearrangement, Baker-Venkataraman rearrangement.

<u>Carbon-nitrogen</u>: Beckmann-, Hofmann-, Curtius-, Lossen- and Schmidtrearrangements. Stevens-, Neber and Benzidine rearrangement,

Carbon-oxygen: Wittig rearrangement, Baeyer-Villiger oxidation.

UNIT-IV 6 h

Chemistry of biological molecules - II

Amino acids and Peptides

Amino acids essential and non essential. Classification and nomenclature of peptides. Sanger and Edman methods of sequencing. Cleavage of peptide bond by chemical and enzymatic methods.

Peptide synthesis- Protection of amino group (Boc-, Z- and Fmoc-) and carboxyl group as alkyl and aryl esters. Use of DCC, EEDQ, HOBt and active esters, in peptide bond formation reactions. Deprotection and racemization in peptide synthesis.solid phase peptide synthesis carbohydrates techniques. Synthesis of oxytocin, and enkephalins.

Vitamins:

7 h

Introduction. Biological importance and synthesis of Vitamin A, Vitamin B_1 (thiamine), Vitamin B_6

(pyridoxine), folic acid, pantothenic acid, riboflavin, Vitamin C, Vitamin E (α -tocopherol), Vitamin H (biotin), Vitamin K₁ and K₂.

SUGGESTED BOOKS

1. Advanced Organic Chemistry – Reactions, Mechanism and Structure, Jerry March,

John Wiley (2008).

2. Advanced Organic Chemistry, F A Carey and R J Sundberg Plenum, (2000).

3. A Guide Book to Mechanism in Organic Chemistry, P Sykes, VI edition, Pearson, (2003).

4. Structure and Mechanism of Organic Chemistry, C. K. Ingold, II Edition, CBS, (2016).

5. Organic Chemistry, R T Morrison, R N Boyd and S K Bhattacharjee, VII edition, Pearson,

(2018).

6. Principles of Organic Synthesis, III edition), R O C Norman and J M Coxon, Blackie

Academic and Professional (Indian Reprint), (2012).

7. Natural Products: their chemistry and biological significance, J Mann, Longman, (2000)

8. Organic Chemistry, Volume I, I L Finar, VI edition, Pearson, (2018).

9. Organic Chemistry, Volume II, I L Finar, VI edition, Pearson, (2018).

10. Organic Chemistry, J Clayden, N Greeves and S Warren, II edition, Oxford University Press,

(2014)

11. Name Reactions – A collection of detailed reaction mechanisms, J J Li Springer, (2012)

12. Modern Methods of Organic Synthesis W Carruthers and I Coldham, IV edition, Cambridge

University Press, (2015).

13. Peptides Chemistry: A practical text book, M. Bodansky, Springer-Verlag NY, (1988).

14. Solid-phase peptide synthesis: A practical Approach-E. Artherton & R.C. Sheppard, I R L,

Oxford Univ. Press, (1989).

15. Peptides: Chemistry and Biology, N Selwad and H.-D. Jakubke, Wiley-VCH, (2002).

C-203: PHYSICAL CHEMISTRY- II

UNIT-I

Thermodynamics-I

Thermodynamics: Concepts of partial molar properties – partial molar free energy, chemical potential, partial molar volume and its significance. Gibbs-Duhem equation, Gibbs-DuhemMargulus equation. Determination of partial molar volume : Graphical method, intercept method and Apparent molar volume method. Concept of fugacity; Determination of fugacity by graphical method and compressibility factor method. Activity and activity coefficient :

Determination of activity coefficient by EMF and solubility method. Thermodynamics of nonideal system-Excess thermodynamic function, GE ,SE , HE etc. Phase Rule : Derivation of phase rule from the concept of chemical potential. Application of Phase Rule to three components system :Principle of triangular diagram : Plots for a mixture of three liquids consisting of one, two and three pairs of partially miscible liquids.

Statistical Thermodynamics: Objectives of statistical thermodynamics, Concept of distributions, Types of ensembles. Thermodynamic probability, Most probable distribution Law – Partition Function, (Definition and significance): Molar and molecular partitions-translational, rotational , vibrational and electronic partition functions- Relation between thermodynamic functions (E, H,S,G and Cv) and the partition functions.

UNIT-II

Thermodynamics-II

Sackur-Tetrode equation for entropy of translation function. Relation between equilibrium constant and partition function. Different Distribution Laws:Types of Statistics : Maxwell – Boltzmann , Bose-Einstein and Fermi-Dirac statistics. Derivation of the equations for above three distribution Laws. Comparision of Bose-Einstein and Fermi-Dirac statistics with Maxwell – Boltzmann statistics. Problems and their Solutions.

Non-equillbriumThermodynamics : Thermodynamic criteria for non-equillbrium states-Phenomenological Laws and Onsager's reciprocity relations, Coupled and Noncoupled reactions, Entropy production and entropy flow. Electro kinetic Phenomenon. Postulates and methodologies: Uncompensated heat and thermodynamics fuction production. deDonder's inequality. Rate of entropy production. Transformations of the generalized fluxes and forces :eg., Chemical reaction, heat flow, Diffusion or material flow, flow of electric current.

UNIT-III

Electrochemistry-I

Elcetrochemistry of solutions: Ionic atmosphere, Debye-Huckel theory for the problem of activity coefficient, Debye-Huckel limiting Law, Debye-Huckel equation for appreciable concentration, Debye-HuckelOnsagar conductance equation and its extension to ion solvent interations, Debye-HuckelBjerrum mode, Ion association, triple ions, triple ions and conductance minima. Thermodynamics of electrified interface, derivation of electro capillary Lipmann's equation, surface excess, thermodynamic aspects of surface excess. The method of determination and measurement of interfacial tension as a function of applied potential difference across the interface.

UNIT-IV

Electrochemistry-II

Structure of electrified interface: Helmholtz theory, Guoy- Chapman theory, Stern model. Overpotential: Concentration, activation and ohmicoverpotential; Derivation of Butler-Volmer equation.

Semiconductor- solution interface: Theory of double layers at semiconductor- electrolyte interface.

Electrocatalysis: Definition and Influence of various parameters. Quantum aspects of charge transfer at electrode solution interface, quantization of charge transfer, tunneling of electrons for hydrogen evolution with reference to electrocatalysis.

Polarography technique-Principle, DME- Merits and limitations, experimental, polarogram, half wave potential, diffusion controlled current, Ilkovic equation (no derivation), qualitative and quantitative estimation of metal ions.

Advanced Electrodes: Rotating disc electrodes, Membrane electrodes (Definition, examples with diagrams and applications to each), carbon electrodes.

SUGGESTED BOOKS

- 1. Molecular thermodynamics, Donald A. Mc Quarrie, John D. Simon University Science Books California, (1999).
- 2. Thermodynamics for Chemists by S. Glasstone, East-West Press, New Delhi, (1960).
- 3. Thermodynamics, by Rajaraman and Kuriacose, East-West Press, (1986).
- 4. Statistical Thermodynamics, M. C. Gupta (Wiley Eastern Ltd.) 1993.
- 5. Elements of Classical and Statistical Thermodynamics, L. K. Nash, Addison-Wiley (1979).
- 6. Thermodynamics, Statistical Thermodynamics and Kinetics by Thomas Engel & Philip Reid, Pearson Education inc. (2007).
- 7. Modern Electrochemistry Vol-1 and 2, J. O. M.Bockrisand A. K. N. Raddy, Plenum, NewYork (1978).
- 8. An introduction to electrochemistry: Samuel Glastone East-West, edition New Delhi (1942)
- 9. 10. Text book of physical chemistry Samuel Glastone, 2nd edition, Mac Millan India Ltd (1991)
- 10. Principles and applications of Electrochemistry- D. R. Crow 3rd edition, Chapmanhall London (1988).
- 11. Phisical chemistry thorugh problems by S K Dogra and S Dogra, Wiley Eastern Ltd., 4thEdn. 1993.
- 12. Electrochemical methods by A J Bard and I R Faulkner,2ndEdn., Wiley New York, 2000.

Ch-204: SPECTROSCOPY-I

UNIT-I

Symmetry and Group Theory in Chemistry

13h

Definition of groups, subgroups, cyclic groups, conjugate relationships, classes, simple theorems in group theory. Symmetry elements and symmetry operations, point groups, Schöenflies notations, representations of groups by matrices, reducible and irreducible representations, characters of representations, Great Orthogonality Theorem (without proof) and its applications, character tables and their uses (representations for the C_n , C_{nv} , C_{nh} , D_{nh} etc groups to be worked out explicitly) Mulliken symbols for irreducible representations

Direct products, Applications of group theory to quantum mechanics- identifying non-zero matrix elements, derivation of the orthonormalization conditions

UNIT-II

Unifying principles

Interaction of electromagnetic radiation with matter- time-dependent perturbation theory,

transition moment integral, selection rules- symmetry and spin forbidden transitions

Infrared Spectroscopy-I

Vibrations of molecules, harmonic and anharmonic oscillators- vibrational energy expression, energy level diagram, vibrational wave functions and their symmetry, selection rules, expression for the energies of spectral lines, computation of intensities, hot bands, effect of isotopic substitution

Diatomic vibrating rotor, Born-Oppenheimer approximation, vibrational-rotational spectra of diatomic molecules, P, Q and R branches, breakdown of the Born-Oppenheimer approximation.

Infrared Spectroscopy-II

Vibrations of polyatomic molecules: Normal coordinates, translations, vibrations and rotations, vibrational

energy levels and wave functions, fundamentals, overtones and combinations Vibrationrotation spectra of

polyatomic molecules- parallel and perpendicular vibrations of linear and symmetric top molecules

Techniques and instrumentation, FTIR

UNIT-III

Raman Spectroscopy

Classical theory of the Raman effect, polarizability as a tensor, polarizability ellipsoids, quantum theory of the Raman effect, Pure rotational Raman spectra of linear and aymmetric top molecules, vibrational Raman spectra, Raman activity of vibrations, rule of mutual exclusion, rotational fine structure- O and S branches, Polarization of Raman scattered photons Structure determination from Raman and IR spectroscopy-AB₂ and AB₃ molecules Techniques and instrumentation

Microwave Spectroscopy

Rotations of molecules, rigid diatomic molecule- rotational energy expression, energy level diagram, rotational wave functions and their symmetry, selection rules, expression for the energies of spectral lines, computation of intensities, effect of isotopic substitution, centrifugal distortion and the spectrum of a non-rigid rotor.

Rotational spectra of polyatomic molecules- linear, symmetric top and asymmetric top molecules Stark effect, techniques and instrumentation

$\mathbf{UNIT} - \mathbf{IV}$

Electronic Spectroscopy

Born-Oppenheimer approximation, vibrational coarse structure, intensities by Franck-Condon principle, Dissociation energy, rotational fine structure, Fortrat diagram, pre-dissociation

.

Electronic structure of diatomic molecules- basic results of MO theory, classification of states by electronic angular momentum- \Box , \Box , \Box , and \Box molecular orbitals, selection rules, spectrum of singlet and triplet molecular hydrogen

Electronic spectra of polyatomic molecules- localized MOs, spectrum of HCHO, change of shape on excitation

Decay of excited states- radiative (fluorescence and phosphorescence) and non-radiative decay, internal conversion

SUGGESTED BOOKS

- 1. Chemical Applications of Group Theory, F. A. Cotton, Wiley Eastern (1976).
- 2. Molecular Symmetry, D. S. Schonland, Van Nostrand (1965).
- 3. Introduction to Molecular Spectroscopy, C. N. Banwell, TMH Edition (1994).
- 4. Introduction to Molecular Spectroscopy, G. M. Barrow, McGraw Hill (Int. Students Edition) (1988).
- 5. Molecular Spectroscopy, J. D. Graybeal, McGraw Hill (Int. Students Edition) (1990).
- 6. Spectroscopy, Vols. 1-3, B. P. Straughan and W. Walker, Chapman Hall (1976).

Ch-205 GREEN SYNTHESIS (SOFT CORE)

36 Hours

12

<u>UNIT-I</u>

Use of ultrasound and Microwaves in organic Synthesis 12 h

Use of ultrasound: Introduction, instrumentation, the phenomenon of cavitation. Sonochemical esterification, substitution, addition, alkylation, oxidation, reduction and coupling reactions.

Use of microwaves: Introduction, concept, reaction vessel/medium, specific effects, atom efficiency (% atom utilization), advantages and limitations. N-alkylation and alkylation of active methylene compounds, condensation of active methylene compounds with aldehydes and amines. Diels-Alder reaction. Deprotection of esters and silyl ethers. Oxidation of alcohols and sulfides.

Ionic-liquids: Introduction, structure, synthesis and applications of some important ionic liquids in organic synthesis.

UNIT-II

Polymer supported reagents in organic synthesis h

Introduction- properties of polymer support, advantages of polymer supported reagents and choice of polymers. Applications. *Substrate covalently bound to the support:* Synthesis of oligosaccharides, Dieckmann cyclisation. Preparation of polymer bound aldehyde and application in aldol and Wittig reactions. Synthesis of polystyrylboronic acid and use in diol protection reaction.

Reagent linked to a polymeric material: Preparation of sulfonazide polymer and application in diazotransfer reaction. Synthesis of polymer bound per acid and its applications.

Polymer supported catalytic reactions: Preparation of polymer supported AlCl₃ and application in etherification and acetal formation reactions.

Phase transfer catalysis and Crown ethers

<u>Phase transfer catalysis</u>: Introduction, definition, mechanism of phase transfer catalysis. Types of phase transfer catalysts and reactions and their Advantages.

Preparation of catalysts and their application in substitution, elimination, addition, alkylation, oxidation and reduction reactions.

<u>Crown ethers</u>: Introduction, nomenclature, features, nature of donor site. General synthesis of Crown ethers.

<u>Synthetic applications</u>: Alkylation, generation of carbenes, aromatic substitution and displacement reactions. Generation and application of superoxide anions. Cation deactivation reactions.

UNIT-III

Multi-component Reactions

12 h

Studies on the mechanistic aspects and use of the following reactions in organic synthesis: Passerini-Ugi; Hantsch; Biginelli; Doebner-Miller; Ritter; Jacobson; Betti; Robinson-Schopf; Barbier; Baylis-Hilmann; Petasis; Ivanov and Suzuki coupling reaction.

SUGGESTED BOOKS

- 1. Some modern methods of Organic Synthesis, W. Caruthers, Cambridge Univ. Press London, 2nd Edition, 1998.
- 2. Organic synthesis: Special techniques, V. K. Ahluwalia and R. Aggarwal, Narosa, New Delhi,2003.
- 3. Green Chemistry, environment friendly alternatives, R. Sanghi and M. M. Srivastava, Narosa, New Delhi, 2003
- 1. Green Chemistry-an introductory text, M. Lancaster, Royal Society of Chemistry, UK, 2003.
- 2. Organic chemistry Vol. 2, 6th Edition, I. L. Finar, Longman, 1992.
- 3. Crown ethers & cryptands, G. W. Gokel, Royal Society of Chemistry, UK, 1991.
- 4. Macrocyclic Polyether Chemistry, G. W. Gokel, S. M. Korzeniowski, Vol 1 to3, Wiley, NY, 1978, 1981,1987.
- 5. Phase Transfer Catalysis in Organic Synthesis, W. B. Weber, G. W.Gokel, Springer, Berlin, 1977.
- 6. Phase Transfer Catalysis, E. V. Dehmlov, S. S. Dehmlov, 2nd Edn., Verlag chemie, Wienheim, 1983.
- 7. Polymers as aids in Organic synthesis, N. K. Mathur, C. K. Narang and R.E. Williams, Academic Press, NY,1980.

INORGANIC CHEMISTRY PRACTICALS (4 days a week, 4 hours a day)

Ch-206 Inorganic Chemistry Practical-III

Gravimetric analysis

- 1. Determination of Fe in iron ore as Fe₂O₃.
- 2. Determination of Ni as nickel dimethylglyoximate in Cu and Ni solution.
- 3. Determination of Ca as CaC₂O₄.H₂O.
- 4. Determination of Al as aluminiumoxinate.
- 5. Determination of Cu as CuSCN in Cu and Fe solution.
- 6. Determination of Zn as ZnNH₄PO₄.

Ch-207 Inorganic Chemistry Practical-IV

Volumetric analysis

- 1. Determination of Ca and Mg in Dolomite solution using EDTA.
- 2. Determination of Cu in Cu and Ni solution iodometrically.
- 3. Determination of Fe in Cu and Fe solution (using $K_2Cr_2O_7$).
- 4. Determination of Cr and Fe in a mixture using ceric ammoniumsulphate.
- 5. Determination of Fe and Al in mixture using EDTA.
- 6. Determination of percentage of Fe and oxalate in K₃Fe(C₂O₄)₃.3H₂O

Suggested Books:

- 1. Vogel's Text book of Qualitative Chemical Analysis, J. Bassett, G. H. Jeffery and J. Mendham, 7th edition, ELBS (2013).
- 2. Vogel's text book of Quantitative Chemical Analysis, 6th Edition, J. Bassett, G. H. Jeffery and J. Mendham, and R. C. Denny, J D Barnes, M.Thomas Prentice Hall (2000)
- 3. Inorganic Semimicro Qualitative Analysis, V. V. Ramanujam; The National Pub. Co. (1990).
- 4. Practical Inorganic Chemistry, G. Marr and B. W. Rockett, Von Nostrand Reinhold Co., London (1972).

5. An Advance course in practical chemistry, A Ghoshal, B Mahapatra and A K Nad; New central

book agency Pvt.Ltd. 3rd eidition 2007.

6. Advanced inorganic analysis, S K Agarwal and Keemtilal; Pragati prakashan, 12th edition 2014.

PHYSICAL CHEMISTRY PRACTICALS (4 days a week, 4 hours a day)

Ch-208 Physical Chemistry Practical -III

1. Study of acid hydrolysis of methyl acetate for two different concentrations of HCl and reporting the relative strength.

2. Study the hydrolysis of methyl acetate in the presence of HCl at two different temperatures and reporting the energy of activation.

3. Determination of dissociation constant of a given indicator by colorimetric method.

- 4. Study of kinetics of autocatalytic reaction between KMnO₄ versus oxalic acid.
- 5. Determination of degree of hydrolysis of aniline hydrochloride at room temperature and calculation of dissociation constant of the base by pH metry.

6. Study of variation of viscosity of a liquid with temperature and determination of the constants A and B.

- 7. Analysis of a binary mixture of two miscible liquids by surface tension method
- 8. Construction of phase diagram of Urea KCl -H₂O system.
- 9. Determination of heat of neutralization of two acids and their relative strength.
- 10. Evaluation of Arrhenius parameter for the reaction between K₂S₂O₈ versus KI (first order)

Ch-209 Physical Chemistry Practical -IV

Conductometry

1.Determination of concentration of mixture of strong acid and weak acid versus strong base.

- 2. Determination of concentration of Weak acid with salt versus strong base.
- 3. Determination of strength of a strong acid, weak acid and a salt versus strong base pH metry

5 Determination of the acidic and basic dissociation constant and isoelectric point of an amino acid by pH metry.

6. Determination of pKa valueor Dissociation constant of phosphoric acid.

7. Determination of pH of acetic acid with sodium acetate buffer. Potentiometry

8. Determination of concentration and amount of $K_2Cr_2O_7$ by titrating against FAS and calculation of redox potential.

9. Determination of concentration of mixture of acids by titrating against NaOH solution.

10.Determination of concentration of KMnO₄by titrating against FAS and calculation of redox potential.

SUGGETED BOOKS

1. Advanced Practical Physical Chemistry by J. B. Yadav, GoelPublications, Meerut (2012).

2. Senior Practical Physical Chemistry by B. C. Kosla, Simla Printers, New Delhi (1987).

3. Experimental Physical Chemistry by Daniel et al., McGraw Hill, New York (1962).

4. Practical Physical Chemistry by A.M James and P. E. Pritchard, Longman's Group Ltd (1968).

5. Experimental Physical Chemistry by Wilson, Newcombe& others, Pergamon Press, New York (1962).

6. Experimental Physical Chemistry by R. C. Behra and B Behra, Tata McGraw, New Delhi (1983).

7. Experimental Physical Chemistry by V. D. Atavale and ParulMathur, New Age International, New York (2001).

8. Practical's in physical chemistry A. Modern Approach by P.S Sindhu, Mac. Millan Publishers, Delhi (2006).

Aliphatic nucleophilic and electrophilic substitution reactions

Nucleophilic substitution reactions:

Substitution at allylic carbon (allylic rearrangement), at a trigonal carbon (hydrolysis of esters and amides, use of DCC in the formation of anhydrides), substitution at a vinylic carbon. Neighboring group participation and S_Ni reactions.

UNIT-I

THIRD SEMESTER

ORGANIC CHEMISTRY SPECIALISATION

CH-301 OC: ORGANIC REACTION MECHANISMS

Electrophilic substitution reactions:

SE2, SE1 and SEi mechanisms. Hydrogen exchange, migration of double bonds, α -halogenation of aldehydes, ketones and acids. Aliphatic diazonium coupling, nitrosation at carbon bearing active hydrogens, diazo transfer reaction, carbene and nitrene insertion, decarboxylation of aliphatic acids, haloform reaction, Haller-Bauer reaction.

UNIT-II

Free-radical chemistry

Generation of free-radicals: Thermal homolysis of peroxides, peresters and azo compounds, photochemical methods.

Free radical reactions: Free-radical mechanisms in general. Free-radical substitution mechanisms. Mechanisms at an aromatic substrate. Neighboring group assistance in free-radical reactions. Reactivity for aliphatic substrates, reactivity at a bridgehead, reactivity in aromatic substrates, reactivity in the attacking radical. Halogenation at an alkyl carbon and an allylic carbon, hydroxylation at an aliphatic carbon, hydroxylation at an aromatic carbon, oxidation of aldehydes to carboxylic acids, formation of hydroperoxides and peroxides, Gomberg-Bachmann reaction, Meerwein arylation, Sandmeyer reaction, Kolbe reaction and Hunsdiecker reaction.

<u>UNIT-III</u>

Photochemistry

Physical and Chemical processes, Jablonski diagram. Photosensitization, quantum efficiency, quantum and chemical yields.

Photochemistry of functional groups:

i) *Olefins*: *Cis-trans* isomerism, [2 + 2]-cycloaddition, rearrangements. Reaction of conjugated olefins; di- π -methane rearrangements (including oxa- and aza- di- π -methane rearrangements). ii) *Ketones*: Excited state of C=O. Norrish type-I and type-II cleavages. Paterno-Buchi reaction. α , β -unsaturated ketones. [2+2] addition. Rearrangement of cyclohexadienones (application in the synthesis of some important natural products).

iii) *Aromatic compounds*: Photorearrangement of benzene and its derivatives, cycloaddition of benzene.

60

11h

10h

52 Hours

iv) *Photochemical oxidations and reductions*: Cycloaddition of singlet molecular oxygen {[2+2], [4+2]-additions}. Oxidative coupling of aromatic compounds, photoreduction by hydrogen abstraction.

Pericyclic reactions-I

Molecular orbital symmetry, Woodward-Hoffmann correlation diagrams. FMO and PMO approaches. Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl system. <u>Electrocyclic reactions</u>: conrotatory and disrotatory motions, 4n, 4n+2 and allyl systems. <u>Cycloadditions</u>: antarafacial and suprafacial additions, $[_{\pi}m_{s} + _{\pi}n_{a}]$ and $[_{\pi}m_{s} + _{\pi}n_{s}]$ -cycloadditions. $[_{\omega}2_{a} + _{\pi}2_{s}]$ and $[_{\pi}4_{s} + _{\omega}2_{s}]$ -cheletropic reactions.

UNIT-IV

Pericyclic reactions-II

Regio, enantio and Endo selectivities in Diels-Alder reactions. Hetero Diels-Alder reaction. <u>Sigmatropic rearrangements</u>: suprafacial and antarafacial shifts of H, sigmatropic shifts involving carbon moieties. [i, j]- sigmatropic rearrangements (including Walk, Claisen, Cope, oxy and aza-Cope rearrangements).

Biochemical mechanisms

Introduction. The mechanistic role of the following in living systems.

- i). Thiamine pyrophosphate (TPP) in decarboxylation of α -ketoacids and in the formation of α -ketols.
- ii). Pyridoxal phosphate (PLP) in transamination, decarboxylation, dealdolisation and elimination reactions of amino acids.
- iii). Lipoic acid in the transfer of acyl group reactions.
- iv). Coenzyme A (CoASH) in the transfer of acyl group.
- v). Biotin and
- vi). Vitamin KH₂ coenzyme in carboxylation reactions.
- vii).Tetrahydrofolic acid (H₄F) in one-carbon transfer reactions.
- viii).Vitamin B₁₂ coenzymes in molecular rearrangement reactions and in the synthesis of methionine and methane.
- ix). Nicotinamide and
- x). Flavin coenzymes in biological redox reactions

SUGGESTED BOOKS

- 1. Advanced Organic Chemistry Reactions, Mechanism and Structure, Jerry March, John Wiley (2008).
- 2. Understanding organic reaction mechanisms, A. Jacob, Cambridge Univ. Press, 1997.
- 3. Introduction to organic chemistry A. Streitweiser, Jr and C. H. Heathcock, Macmillan, 1985.
- 4. Physical and mechanistic organic chemistry, R.A.Y. Jones, 1st Edn. Cambridge Univ. Press, 1979.
- 5. Mechanisms of molecular migrations, Vols I and II, B. S. Thiagarajan, 1st Edn. Pergamon Press, Oxford, 1979.
- 6. P. J. Garratt in Comprehensive organic chemistry, D. Barton and W. D. Ollis, 1st Edn. Pergamon Press, Oxford, 1979.
- 7. Radicals in organic synthesis, B. Giese, Pergamon Press, 1986.

10h

5h

- 8. Stereoelectronic effects in organic chemistry, P. Deslongchamps, 1st Edn. Pergamon Press, 1983.
- 9. Frontier orbitals and organic chemical reactions, Ian Fleming, John Wiley, 1980.
- 10. Molecular orbital theory for organic chemistry, A. Streitweiser, 1st Ed. Wiley & Sons, NY, 1969.
- 11. Organic photochemistry, J. M. Coxon and B. Halton, 1st Edn, Cambridge Univ. Press, London, 1974.
- 12. Orbital symmetry, R. E. Lehr and A. P. Marchand, Academic Press, 1972.
- 13. Molecular reactions and photochemistry, C. H. Deputy and D. S. Chapman, 1st Edn. Prentice-hall India, New Delhi, 1972.
- 14. Stereochemistry of Organic Compounds: Principles and Applications, D Nasipuri, New-Age International, (1999).
- 15. Biochemistry, G. Zubey, Macmillan, NY, 1998.
- 16. Biochemistry, D. Voet and J. G. Voet, John Wiley & Sons, 1998.
- 17. Principles of Biochemistry, A. L. Lehninger, D. L. Nelson & M. M. Cox, 2nd Edn. Worth Publishers, NY, 2005.

CH-302 OC CHEMISTRY OF NATURAL PRODUCTS

52 Hours

<u>UNIT-I</u>

Terpenoids and Carotenoids

Classification, nomenclature, occurrence and isolation. Isoprene rules.

Stereochemistry of citral, farnesol, limonene, 1,8-cineole, menthols and borneols. Correlation of configurations of terpenoids.

Structure elucidation of camphene, α -pinene, β -caryophyllene, α -santonin and gibberrillic acid. Synthesis and biosynthesis of the following:

Linalool, α -terpineol, fenchone, eudesmol, abietic acid.

Commercial synthesis of camphor.

Biosynthesis of squalene and cyclisation of squalene into α -lanosterol and friedelene. <u>Carotenoids</u>: Methods of isolation. Structural relationship of α -, β - and γ -carotenes. Structure elucidation and synthesis of β -carotene.

<u>UNIT-II</u>

Alkaloids

Definition, nomenclature, occurrence, isolation, classification, General methods of structure elucidation. Synthesis and biosynthesis of the following alkaloids:

Ephedrine, hygrine, coniine and cocaine.

Cinchona alkaloids: Cinchonine and quinine.

Opioid alkaloids: Morphine, codeine, thebiene and heroin.

Structure elucidation and synthesis of papaverine, reserpine and ergotamine.

Photochemical synthesis of Nuciferine, coradyline and tylophorine.

UNIT-III

Porphyrins and vitamin B₁₂

Structure elucidation and synthesis of haemin, chlorophyll-a and vitamin- B_{12} (synthesis of Vitamin- B_{12} from cobyric acid).

Nucleic acids

Introduction, components of nucleic acids, nucleosides, nucleotides and oligonucleotides. Structure elucidation and synthesis of nucleosides and nucleotides.

Chemical synthesis of oligonucleotides: Protecting groups for hydroxy group in sugar, amino group in the base and phosphate functions. Methods of formation of internucleotide bonds: DCC, phosphodiester approach, phosphotriester approach, phosphite triester and phosphoramidite methods. Solid phase synthesis of oligonucleotides.

7h

12h

8h

UNIT-IV

Prostaglandins

Introduction, nomenclature, classification and biological role of prostaglandins. Structure elucidation and stereochemistry of PGE_1 , PGE_2 and PGE_3 . Synthesis of PGE_1 and PGE_2 by Corey's and Stork's approaches. Synthesis of PGE_3 by Upjohn's approach. Synthesis of prostacyclin I_2 and thromboxane B_2 . Biosynthesis of prostaglandins.

Insect pheromones

Introduction, classification. Pheromones in pest control.

Syntheses of (one synthesis should be stereoselective synthesis)

- i) Grandisol (component of boll weevil pheromone)
- ii) Farenal (trail pheromone of pharaoh's ants)
- iii) Brevicomin (pheromone from *Dendroitis brevicomis*)
- iv) (+)- Disparlure (gypsy moth sex pheromone).
- v) 3,11-Dimethy1-2-nonacosanone (pheromone of German cockroaches).
- vi) Bombykol (sex pheromone of silkworm moth).
- vii) Multistriatin (Elm bark beetle sex pheromone).

SUGGESTED BOOKS

- Natural products: Their chemistry and biological significance-J. Mann,
 R. S. Davidson, J. B. Hobbs, D. V. Banthorpe & J. B. Harborne, Longman, UK, 1994.
- 2. Terpenes, J. Verghese, Tata McGraw-Hill, New Delhi, 1982.
- 3. Chemistry of terpenes and terpenoids, A. Newman, Academic Press, London, 1975.
- 4. Handbook of naturally occurring compounds Vol. II: Terpenes, T. K. Davon, A. I. Scott, Academic Press, NY, 1972.
- 5. Natural products chemistry Vol. I & II, K. Nakanishi, T. Goso, S. Ito, S. Natori & S. Nozoe, Academic Press, NY, 1974.
- 6. Total synthesis of natural products Vol. I & VI, Apsimon, John Wiley, NY, 1973-1981.
- 7. Organic chemistry Vol.II, I. L. Finar, 6th Edn. Longman, 1992.
- 8. Chemistry of natural products Vol. I & II, O. P. Aggarwal, Goel Publishing House, 6th Edn. 1982.
- 9. Total synthesis of natural products: The chiral approach Vol.III, S. Hanessian Pergamon Press, 1983.
- 10. Total synthesis of steroids, Akhaun & Titov, Jerusalem, 1969.
- 11. Medicinal natural products: A biosynthetic approach, P. M. Dewick. John Wiley, Chichester, 1997.
- 12. The colours of life: An introduction to the chemistry of porphyrins and related compounds, L. R. Milgrom, Wiley Chichester, 1995.
- 13. Interpretation of the UV spectra of natural products, A.I. Scott, Pergamon Press, Oxford, 1964.
- 14. Spectral data of natural products Vol. I- K. Yamaguchi, Elsevier Publishing Co, London, 1970.
- 15. Chemistry of natural products: A unified approach, N. R. Krishnaswamy, University Press, India, 1999.

7h

CH-303: OC: ORGANIC SPECTROSCOPY

<u>UNIT-I</u>

Ultraviolet and visible spectroscopy

Classification of elecgronic transitions, Terminology, Substituent and solvent effects, UV spectral study of alkenes, polyenes, enones and aromatic compounds. Empirical rules for calculating λ_{max} .

Vibrational Spectroscopy: spectroscopy

Sampling techniques, Group frequencies, factors affecting group frequencies, Bond order, Mass effect, Conjugation, Inductive, resonance, steric effects. Intramolecular interactions. Applicaton of IR in the stuy of H-bonding, stereoisomerism and tautomerisam. Complimentarity of IR and Raman. Identification of the following organic compounds by IR: Alkanes, Alkenes, Alkynes,

Aromatic compounds, Aldehydes, Ketones, Alcohols, Acids, Acid chlorides, Amides, Amines, Esters, Halides, Nitro compounds, etc., problems using UV and IR.

<u>UNIT-II</u>

Nuclear magnetic resonance spectroscopy-I

Introduction, Magnetic properties of nuclei- Resonance condition. Nuclear spin, population of nuclear spin levels and NMR isotopes, Relaxation methods. Insturmetnation and sample handling, FT-NMR.

Chemical shift. Mechanism of shielding and deshielding in Alkanes, Alkyl halides, Alkenes, Aromatic compounds, Carbonyl compounds and Annulenes. Pascal's triangle-low and high resolution, spectrum of ethnaol. Karplus Curve, Diamagnetic and paramagnetic effects and magnetic anisotropy. Equivalence of protons-chemical and magnetic equivalence. Spin-systems: First order and second order coupling of AB systems, Simplifications of complex spectras.

Problems.

Spin-spin interactions: AX,AX₂, AX₃, AMX,AB types. Vicinal, geminal and long range coupling-Spin decoupling. Chemical shift reagents and deuterium exchange. Stereochemistry and hindered rotations. Temperature effects.

UNIT-III

Nuclear magnetic resonance spectroscopy-II

CIDNP, Nuclear Overhauser effect (NOE). Factors influencing coupling constants and Relative intensities. Protons attached to elements other than carbon.

¹³C NMR Spectroscopy: Range and factors affecting chemical shifts of alkanes, alkyl halides, alkenes, alcohols, ethers, alkynes, carbonyl compounds and aromatics..

Multiple resonance spectroscopy: Introduction to 2D-techniques: DEPT, COSY, HETCOR, and INADEQUATE.

Explanation of the principle, applications to structure elucidation and stereochemistry of simple organic molecules.

Dynamic NMR.

NMR spectroscopy of other nuclei with spin I = $\frac{1}{2}$. Introduction to ^{15}N , ^{19}F , ^{29}Si and ^{31}P NMR spectroscopies. Chemical shift values for ^{15}N , ^{19}F , ^{29}Si and ^{31}P containing compounds.

52 hours

6h

9h

13h

UNIT-IV

Mass spectrometry and Composite Prooblems:

Basic principles-instrumentation – ion production-ion analysis-magnetic sector instruments Quadrapole mass spectrometers. Time of flight mass spectrometers-ion cyclotron resonance spectrometers- Mass spectrum-molecular ion-types of ions in mass spectra and effects of isotopes on mass spectra. Methods of ionization, EI, FAB mass and MALDI methods. Fragmentation of Alkanes, Alkenes, alkyl halides, alcohols, aldehydes, ketones, acids, esters, ethers, amines, nitro and halo compounds peptides, Nitrogen rule, Factors affecting cleavage patterns. MeLafferty and MeLafferty +1 rearrangment. Determination of molecular formula. Composite problems.

Use of HRMS to determine exact molecular formulae of compounds.

Application of UV, IR, NMR and MS methods and chemical reactions in the structure elucidation of organic compounds. 5h

SUGGESTED BOOKS

- 1. Applications of absorption spectroscopy to organic compounds, J. R. Dyer, Prentice-Hall, New Delhi, 1969.
- 2. Organic spectroscopy, P. Laszlo and P. Stang, Harper & Row, New York, 1971.
- 3. Organic spectroscopy, W. Kemp, ELBS London, 2000.
- 4. Spectrometric identification of organic compounds, R. M. Silverstien, and W. P. Weber, 2005.
- 5. Introduction to spectroscopy, 3rd Edn., D. L. Pavia, G. M. Laupman and G. S. Kriz, Harcourt College Publishers, 2001.
- 6. Organic mass spectroscopy, K. R. Dass & E. P. James, IBH New Delhi, 1976.
- 7. Interpretation of organic mass spectra, F. W. McLafferty, W. A. Benjamin, London, 1973.
- 8. Practical Organic Mass Spectroscopy, 2nd Edn. J R Chapman, John Wiley, NY, 1993.
- 9. The IR Spectra of complex molecules, Vols. I and II, L J Bellamy, Chapman and Hall, London, 1975.
- 10. Spectroscopic techniques for Organic Chemists, J W Cooper, John Wiley, NY, 1980.
- 11. Biomolecular NMR Spectroscopy, J N S Evans, Oxford Univ. 1995.
- 12. Mass spectrometry a foundation course, K Downard, RSC, Cambridge, 2004.
- 13. Mass spectrometry of organic compounds, H. Budzkiewicz, Djerassi C. and D. H. Williams, Holden-Day New York, 1975.
- 14. Modern NMR techniques and their Applications, Ed. A I Popov, Marcel Deckker, 1991.
- 15. Modern structural theory of organic compounds, L. N. Ferguson, Prentice-Hall, New Delhi, 1973.
- 16. Instrumental methods of analysis, H. H. Willard, L. L. Merrit, J. A. Dean and F.A. Settle, CBSPublishers and Distributors, 1986.
- 17. Fundamentals of molecular spectroscopy, 4th edn., C. N. Banwell and E. M. McCash, Tata McGraw-Hill, New Delhi, 1999.

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ORGANIC CHEMISTRY PRACTICALS (4 days a week, 4 hours a day)

CH-306 Organic Chemistry Practical-I

Preparation (one stage)

- 1. Cannizarro reaction: Benzaldehyde.
- 2. Fries rearrangement: Phenyl acetate.
- 3. Friedel-Crafts reaction: Benzene and Acetyl chloride.
- 4. Sandmeyer reaction: 4-Chlorotoluene from 4-toluidine.
- 5. Pechmann reaction: Resorcinol and ethylacetoacetate.
- 6. Oxidation of Cyclohexanol.
- 7. Preparation of S- Benzylisothiuronium chloride.
- 8. Synthesis of *p*-iodonitrobenzene
- 9. Synthesis of N-Phenyl-2,4-dinitroaniline.
- 10. Synthesis of 2,4,6-tribromoaniline.
- 12. Synthesis of 2,4-dichlorophenoxyacetic acid.

CH-307 Organic Chemistry Practical-II

Qualitative analysis

Systematic analysis and identification of organic compounds.

CH-308 Organic Chemistry Practical – III

Preparation (Two and three stages)

- 1. 2,4-Dinitrophenylhydrazine from chloronitrobenzene.
- 2. Anthranilic acid from phthalic acid.
- 3. Benzanilide from benzophenone.
- 4. Benzilic acid from benzoin.
- 5. Synthesis of Acridone.
- 6. Synthesis of Hydantoin.

CH-309 Organic Chemistry Practical-IV

Quantitative analysis

- 1. Titrimetric estimation of amino acids.
- 2. Saponification value of oil.
- 3. Estimation of glucose by Feighling's method.
- 4. Estimation of keto group.
- 5. Estimation of phenols.
- 6. Iodine value of oil (chloramine-T method).

- 1. Laboratory manual of Organic Chemistry- B. B. Dey, M V Sitaraman and T R Govindachari, Allied Publishers, New Delhi, (1996).
- 2. Practical Organic Chemistry Mann and Saunders, (1980).
- 3. Text Book of Practical Organic Chemistry- A. I. Vogel, (1996).

- 4. Test Book of Quantitative Organic Analysis- A. I. Vogel, (1996).
- 5. A Handbook of Organic Analysis Clarke and Hayes, (1964).
- 6. Comprehensive practical organic chemistry : Preparation and quantitative Analysis, V. K. Ahluwalia, R. Aggarwal, Universities Press (India), 2000.
- 7. Comprehensive practical organic chemistry: Qualitative analysis, V. K. Ahluwalia, S. Dhingra, Universities Press (India), 2000.
- 8. An advanced course in practical chemistry, A. Ghoshal, B. Mahapatra and A. Kr. Nad, New central book agency, Calcutta, 2000.
- 9. Advanced practical organic chemistry, J. Mohan, Vol. I and II, Himalaya Publishing House, 1992.
- 10. Practical organic chemistry (Quantitative analysis), B. B. Dey, M. V. Sitaraman and T. R. Govindachari, Allied Publishers, New Delhi, 1992.

FOURTH SEMESTER ORGANIC CHEMISTRY SPECIALIZATION

CH-401: OC: ORGANOMETALLIC AND HETEROCYCLIC CHEMISTRY

UNIT-I

Organometallic Compounds in Organic Synthesis-I

Chemistry of Organotransition metal complexes:

General introduction. 18- and 16-Electron rules. General rules.

Complexation and De-complexation Reactions: s-Bonded systems including h1 ligands. p-
Bonded systems involving dihapto to octahapto ligands such as- olefins, acetylenes, allyl
moieties, butadiene, cyclobutadiene, arenes, cyclopenta, cyclohexa and cycloheptadienyl
moieties; cyclohepta, cyclooctatrienes, and cyclooctatetraene moieties.4hUse of organotransition metal complexes as protecting and stabilizing groups: Protection of
olefins, acetylenes and dienes. Stabilization of cyclobutadines and norbornadienones.4hOrganometallics as electrophiles and nucleophiles: Nucleophilic addition to h2, h5 and h6
complexes. Electrophilic addition to h4, h6 and carbene complexes.3hOrganometallics in coupling and cyclization reactions: Coupling and cyclization of organic
nucleophiles with olefins (including Heck reaction), and coupling of olefins with acetylenes
(including Felkin's reaction).3h

Organometallics in isomerization, oxidation and reduction reactions: Isomerization of olefins, allylic alcohols and allylic ethers. Oxidation of olefins (including Wacker's process and epoxidation) and reduction of olefins and α,β -unsaturated compounds (including Wilkinson's reaction).

UNIT-II

Organometallic Compounds in Organic Synthesis-II

Carbonylation reactions:

Use of zirconium complexes in the synthesis of esters, acids, aldehydes or acyl halides from alkyl halides and in the hydroformylation of olefins and dienes.

Use of iron complexes for the insertion of CO group into organic molecules such as dienes, alkyl halides, and vinyl epoxides.

Use of cobalt complexes in the synthesis of ketones from epoxides, lactones from allylic alcohols and in the hydroformylation of olefins.

Use of palladium complexes for the carbonylation of alkyl halides, dienes and allenes.

4h

52 Hours

Application of the following organometallics in Organic Synthesis:

Organozincs: Preparation, reaction with compounds containing acidic protons, reaction with C-C multiple bonds, trans-metallation, addition reactions of zinc reagents with carbonyl compounds. Simmons Smith, and Reformatsky reaction. *Organolithiums*: Preparation. Deprotonation reactions, nucleophilic addition reactions, reactions with imines, nitriles and isonitriles. *Organocopper reagents*: (Gilman reagents-lithium dialkyl cuprates): Preparation,

Organocopper reagents: (Gilman reagents-lithium dialkyl cuprates): Preparation, reactions with alkyl, allyl, vinyl, benzyl and aryl halides, aldehydes, ketones (including a,b-unsaturated carbonyl compounds) and epoxides.

Organoseleniums: preparation. Use of organoseleniums in the synthesis of alkenes fromalkyl halides, α,β -unsaturated carbonyl compounds from carbonyl compounds. *Organotelluriums*: Debromination of vic-dibromides, deoxygenation of epoxides, oxidation of hydroquinone and synthesis of biaryls.

Organoaluminiums: Preparation, hydroalumination and carboalumination of alkenes. Nucleophillic addition reactions with carbonyl compounds and Hydrocyanation. Preparation of alkenyldialkylalanes and their reactions.

4h

UNIT-III

Organometallic Compounds in Organic Synthesis-III

Organosilicons: Introduction, preparation and general reactions of trialkylsilyl halides. Peterson olefination.

Organotins: Preparation and reactions of tri-*n*-butyltin hydride, Barton decarboxylation and Barton- McCombie reaction.

Organocerates: Preparation and reactions of organocerates.

Organomercurials: Preparation. Electrophilic substitution reactions. Solvomercuration-demercuration and cyclopropanation of alkenes. 4h

Heterocyclic Chemistry-I

Small ring heterocycles: Properties and reactions of 3- and 4- membered heterocycles:-	
oxiranes, thiranes, aziridines, azetidines, oxetanes and thietanes.	4h
Benzo-fused heterocycles: Synthesis and reactions of benzofurans, benzothiophenes,	
benzoxazoles, benzothiazoles and benzimidazoles.	3h
Six-membered heterocycles with two or more heteroatoms: Synthesis of Diazines, triazines	5,
tetrazines and thiazines.	2h

UNIT-IV

Heterocyclic Chemistry-II

Seven and large membered heterocycles: Synthesis and reactions of azepanes, oxepines, thiepines, diazepines, thiazepines, azocines, diazocines, dioxocines and dithiocines.

	4n
Heterocycles containing P, As, Sb and Bi: Synthesis of 5- and 6- membered	
heterocycles with P, As, Sb and Bi.	3h
Mesoionic compounds: General classification, chemistry of some important meso-ionic	
heterocycles of type-A and type-B and their applications	6h

SUGGESTED BOOKS

- 1. Organometallic Chemistry, R. C. Mehrotra and A. Singh, Wiley Eastern, 1991.
- 2. The Organometallic Chemistry of the transition metals, R. H. Crabtree, 1988.
- 3. Principles and application of the organotrnsition metal chemistry, J. P. Collman, L. S. Hegedus, University Science books, 1980.
- 4. An introduction to Organometallic Chemistry, A. W. Parkins and R. C. Poller, Macmillan, 1986.
- 5. Modern Synthetic Reactions, H. O. House, W.A. Benjamin, California, 2nd Edn. 1972.

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- 6. Organometallics, Vol. 1 & 2, M. Bochmann, Oxford Chemistry primers, Oxford University Press, 1994.
- 7. Advanced Organic Chemistry, J. March, 4th Edn. John Wiley, 2008.
- 8. Organotransition metal chemistry, S. G. Davies, Pergamon Press, Oxford, 1982.
- 9. Heterocyclic Chemistry, Vols. 1-3, R. R. Gupta, M. Kumar and V. Gupta, Springer Verlag.
- 10. The Chemistry of Heterocycles, T. Eicher and S Hauptimann, Thieme.
- 11. Heterocyclic Chemistry, J. A. Joule, K. Mills and G. F. Smith, Chapman and Hill.
- 12. Heterocyclic Chemistry, T. L. Gilchrist, Longman Scientific Tech.
- 13. Contemporary Heterocyclic Chemistry, G. R. Newkome, and W. W. Paudler, Wiley-Inter Science.
- 14. An introduction to Heterocyclic Compounds, R. M. Acheson, John Wiley.
- 15. Comprehensive Heterocyclic Chemistry, A. R. Katritzky and C. W. Rees, Eds. Pergamon Press.
- 16. Stereochemistry of Organic Compounds, D Nasipuri, New-Age International, (1999).

CH-402 OC STEREOCHEMISTRY AND RETROSYNTHETIC ANALYSIS **52 Hours**

STEREOCHEMISTRY

UNIT-I

Optical activity in the absence of chiral atoms

Chirality in biphenyls, adamentanes, ansa compounds, cyclophanes, *trans*-cyclooctene, catenanes, rotaxanes and helicenes. Assignment of R, S- configuration to these classes of compounds.

Optical activity due to the presence hetero atoms

Chirality of organic compounds due to the presence of silicon, nitrogen, phosphorous, arsenic and sulphur atoms. Determination of R.S-configuration of these compounds using CIP rules.

Transannular reactions

Conformational analysis of medium rings.

Trasnannular reactions: Hydrolysis of medium ring epoxides and bromination of C₈–C₁₀ cyclic dienes.

UNIT-II

Determining absolute and relative configuration

i). Chemical correlation of configuration: Methods without involving the chiral centre. Chemical transformation involving the chiral centre. Chemical correlation involving diastereomers. ii). Methods based on comparison of optical rotation: Distance rule, Rule of shift, Rule of optical superposition, Mill's rule, Method based on molecular rotation difference

iii) The method of quasi-racemate.

iv). Use optical rotatory dispersion curves: α -axial haloketone rule and its applications, octant rule (application of these rules in the determination of absolute configuration of substituted cyclohexanones, decalones and cholestanones).

v). Method based on anomalous X- ray scattering.

RETROSYNTHETIC ANALYSIS

Disconnection approach

Introduction to synthons, and synthetic equivalents, disconnection approach. Basic principles and terminologies used in disconnection approach. One group C-X and two group C-X disconnections. Chemoselectivity, reversal of polarity, cyclisation reactions.

UNIT-III

Protecting groups

Principle of protection of alcohols, amines, acids and carbonyl groups

C-C one group and C-C two group disconnections

Synthesis of alcohols, carbonyl compounds and alkenes. Use of acetylides and aliphatic nitro compounds in organic syntesis. Diels-Alder reaction, 1,3-difunctionalised compounds, α , β -

6h

10h

5h

4h

3h

4h 10h unsaturated compounds, carbonyl compounds condensations, 1,5- difunctionalised compounds. Micheal addition and Robinson annelation.

UNIT-IV

Ring Synthesis

4h

Synthesis of saturated heterocycles and 3-, 4-, 5- and 6-membered rings.Synthesis of some complex molecules using disconnection appoach6hAromadendrene, longifloene, cortisone, reserpine, vitamin-D, juvabione, fredericamycin-A and
Lycorane.

- 1. Stereochemistry of carbon compounds, E. L. Eliel, S. H. Wilen and L. N. Mander, John Wiley & Sons, 1994.
- 2. Stereochemistry, Potapov, MIR, Moscow, 1984.
- 3. Stereochemistry, Nasipuri, D, New Age, 1999.
- 4. Advanced organic chemistry, J. March, 4th Edn. John Wiley, 2008.
- 5. Organic Chemistry, R. E. Ireland Prentice-Hall India, New Delhi, 1975.
- 6. Some modern methods of Organic Synthesis, W. Caruthers, Cambridge Uni. Press London, 2nd Edn., 1998.
- 7. Stereochemistry of organic compounds- Principle and applications, D. Nasipuri, 2nd Edn., New Age International Publishers, 2001.
- 8. Organic synthesis: The synthon approach, S. Warren, John Wiley & Sons, New York, 1st. Edn. 1983.
- 9. Designing organic synthesis: A disconnection approach, S. Warren, John Wiley & Sons, New York, 2nd Edn. 1987.
- 10. Organic synthesis, C. Willis and M. Wills, Oxford University Press, 1995.
- 11. Organic synthesis: Concepts, methods and starting materials, J. Furhfop and G. Penzillin, Verlag VCH.
- 12. Principles of organic synthesis, R. Norman and J. M. Coxon, Blackie Academic & Professional.
- 13. Advanced organic chemistry Part B, F. A. Carrey and J. Sundberg, Plenum Press, 1999.
- 14. Organic chemistry Vol. 2, 6th Edn., I. L. Finar, Longman, 1992.

CH-403 OC ORGANIC SYNTHESIS

UNIT-I

C-C and C-N bond forming reactions

Darzen's reaction, Use of acetylides in C-C bond formation reactions. Acid-catalyzed self condensation of olefins, Prins reaction, Shapiro reaction, Dieckmann cyclization, Robinson Hofmann-Loeffler-Freytag reaction. annulations, Hofmann-Martius reaction. Acyloin condensation. Houben-Hoesch reaction.

Stork-enamine synthesis. Meyer synthesis. Use of nucleophilic nitrogen and electrophilic carbon (NH₃, amines and nitrite as nucleophiles in substitution, NH₃ and amines in addition to ketones and aldehydes) and electrophilic nitrogen and nucleophilic carbon (nitration, nitrosation) for the bond formation reactions (including Chichibabin reaction, Skraup synthesis, Mitsunobu reaction, N-Nitroaromatic amine rearrangement, Fisher-Hepp reaction. Japp- Klingemann reaction).

UNIT-II

Reagents in organic synthesis

Use of the following in organic synthesis and functional group tansformations. Aluminium iso-propoxide, NBS, LDA, DCC, DDQ, Corey-Chaykovsky reagent, Raney-Nickel, diazomethane, TMS-chloride, 1,3-Dithiane (reactivity and umpolung), PPA, Yamaguchi reagent. Woodward and Prevost hydroxylation.

Oxidations-I

Cr (VI) oxidants, Mn (VII) oxidants, OsO₄, SeO₂, Pb (OAc)₄, HIO₄, Ag₂O, DMSO.

Oxidations-II

ozone, peroxides (H₂O₂, t-BuOOH, dibenzoylperoxide) and peracids (Preparation, properties and applications of CF₃COOOH, *m*-CPBA, momoperphthalic acid) as oxidizing agents. Dess-Martin oxidation.

UN<u>IT-III</u>

Reductions

Complex metal hydrides, dissolving metal reductions (including Birch, Benkeser, Clemmensen reductions), diimide reduction, catalytic hydrogenation (homogeneous and heterogeneous), organoboranes as reducing agents. Wolf-Kishner reduction, McMurry reaction. Pummer, Willgerdot, Corey-Bakshi-Shibata and Tishchenko reactions.

UNIT-IV

Asymmetric Synthesis

'ee' and methods of determination of 'ee'. Stereoselectivity: classification, terminology and principle. Asymmetric synthesis and asymmetric induction. Double diastereoselection and double asymmetric induction. Acyclic stereoselection: Addition of nucleophiles to carbonyl compounds (1,2-1,3- and 1,4asymmetric induction). Asymmetric aldol condensation. Addition of allylmetal and allylboranes to carbonyl group.

12h

52 Hours

4h

9h

15h

5h

Diastereoselection in cyclic systems: Nucleophilic addition to cyclic ketones (formation of axial and equatorial alcohols, catalytic hydrogenation, alkylation, diastereoselective oxidations and stereoselective cyclization of poylenes).

Enantioselective synthesis: Reduction with chiral hydride donors [(S)-PBMgCl, (-)-

ⁱBOA1Cl₂, alpine-borane, (S)-BINAL-H, (R,R)-DIOP, and (S,S)-CHIRAPHOS).

Enantioselective alkylation of ketones via hydrazones. Enantioselective alkylation with chiral PTC. Enantioselective Michael addition. Enantioselective intramolecular aldol

condensation. Use of (+)- and (-)- DET in asymmetric epoxidation.

Polymer-bound chiral catalysts in asymmetric induction.

Asymmetric amplification.

- Advanced organic chemistry, J. March, 4th Edn. John Wiley, 2008. 1. Organic synthesis, R.E.Ireland, Prentice-hall India, New Delhi, 1975.
- Understanding organic reaction mechanisms, A. Jacob, Cambridge Univ Press, 1997. 2.
- 3. Introduction to organic chemistry, A. Streitweiser, Jr and C. H. Heathcock, Macmillan, 1985.
- Physical and mechanistic organic chemistry, R. A.Y. Jones, 1st Edn. Cambridge Univ 4. Press, 1979.
- Modern synthetic reactions, H. O. House, W. A. Benjamin, California, 2nd Edn. 1972. 5.
- Some modern methods of organic synthesis, W. Carruthurs, Cambridge Univ. Press, 6. London, 2nd Edn. 1978.
- Mechanisms of molecular migration, Vols I & II, B.S. Thyagarajan, Pergamon Press, 7. Oxford, 1979.
- Comprehensive organic chemistry, D. Barton and W. D. Wallis, Pergamon Press, 8. Oxford, 1983.
- 9.
- Organic chemistry Vol. II, I. L. Finar 6th Edn. Longman, 1992. Organic reaction Mechanisms, 3rd Edn., V. K. Ahluwalia and R. K. Prashar, Narosa, New 10. Delhi. 2005.

CH-404 OC MEDICINAL ORGANIC CHEMISTRY

52 Hours

<u>UNIT-I</u>

Pharmacokinetics, Pharmacodynamics, Theories of drug activity& Drug design

Basics of drug receptor interactions. Theories of drug activity. Hansch equation. Computer-aided drug design and molecular modeling. **4h**

<u>Steroids</u>

Occurrence. Nomenclature, basic skeleton, Diels hydrocarbon and stereochemistry. Isolation, structure and structural elucidation of sterols and bile acids (determination of ring size, nature of side chain, position of angular methyl and stereochemistry of ring junctions). Sex hormones and corticosteroids. Synthesis of cholesterol, estrone, progesterone, androsterone, testosterone. Photo products of ergosterol- vitamins D. Barton reaction for the synthesis of aldosterone.

Marker degradation. Brief discussion of homosteroids, norsteroids and oral contraceptives. Synthesis of (dl)-norgestrel and ethinyl oestradiol. 13h

UNIT-II

<u>Antibiotics</u>

Structure elucidation and synthesis of streptomycin, penicillins, cephalosporin-C, chloromycetin and tetracyclins (terramycin and aureomycin). **10h**

UNIT-III

<u>Mechanism of drug action and synthesis of the following classes of drugs, with recent</u> <u>developments:</u>

Antipyretics, analgesics and non steroidal anti-inflammatory drugs: Aspirin, paracetamol, phenacetin, novalgin, phenylbutazone and ibuprofen.

Antidiabetics: Sequence of A- & B- chains of insulin, glibenclamide, metformin, ciglitazone. *Antihistamines*: Methapyrilene, chlorpheniramine.

Antivirals : Acyclovir, amantidine, rimantidine and zidovudine.

Antineoplastic agents: Introduction, cancer chemotherapy, special problems, role of alkylating agents and antimetabolites in treatment of cancer. Mention of carcinolytic antibiotics and mitotic inhibitors. Synthesis of mechlorethamine, cyclophosphamide, melaphan, uracil mustards and 6-mercaptopurine. Recent development in cancer chemotherapy. Hormone and natural products. *Cardiovascular drugs:* Introduction, cardiovascular diseases, drug inhibitors of peripheral sympathetic function, central intervention of cardiovascular output. Direct acting arteriolar dilators. Synthesis of amyl nitrite, sorbitrate, diltiazem, quinidine, verapamil, methyldopa, atenolol, oxyprenol.

UNIT-IV

Local anti-infective agents:

Introduction and general mode of action. Synthesis of sulphonamides, furazolidone, nalidixic acid, ciprofloxacin, dapsone, aminosalicyclic acid, isoniazide, ethionamide, ethambutal, fluconazole, econozole, griseofulvin, chloroquin and primaquin.

Psychoactive drugs- chemotherapy of the mind:

Introduction, neurotransmitters, CNS depressants, general anaesthetics, mode of action of hypnotics, sedatives, anti-anxiety drugs, benzodiazepines, buspirone, neurochemistry of mental diseases. Antipsychotic drugs- the neuroleptics, antidepressants, butyrophenones, serendipity and drug development, stereochemical aspects of psychotropic drugs. Synthesis of chlorpromazine, diazepam, oxazepam, chlorazepam, alprazolam, phenytoin, ethosuximide, trimethadione, barbiturates, thiopental sodium, glutethimide. **12h**

- 1. Burger's Medicinal Chemistry and Drug Discovery, Vols. 1-6 Ed. D.J. Abraham, John Wiley, 2003
- 2. Foye's Principles of Medicinal Chemistry, 6th Edn., T L Lemke and D A Williams Eds., Lippincott, Williams and Wilkins, 2007
- 3. An Introduction to Medicinal Chemistry, P Graham, III Ed., Oxford, 2006
- 4. Medicinal Chemistry, N Weaver, Oxford, 2006
- 5. Goodman and Gilman's Pharmacological Basis of Therapeutics, 11th Edn., Tata McGraw-Hill, 2005.
- 6. The Organic Chemistry of Drug Design and Drug Action, R B Silverman, II Edn, Academic Press, Amsterdam, 2004.
- 7. Wilson and Gisvold's Text Book of Organic Medicinal and Pharmaceutical chemistry, J H Block and J M Beale, Jr., Eds., Lippincott, Williams and Wilkins, 2003.
- 8. Medicinal Chemistry G R Chatwal, Himalaya, New Delhi, 2002
- 9. Instant Notes Medicinal Chemistry, P Graham, Viva, New Delhi, 2002
- 10. Medicinal Chemistry, A Kar, Wiley, 2000.
- 11. An Introduction to Drug Design, S.S. Pandey and J.R. Dimmock, New Age International, 1999.
- 12. Strategies for Organic Drug Synthesis and Design, D. Lednicer, John Wiley, 1998.
- 13. Synthetic drugs, G. R. Chatwal, Himalaya, New Delhi, 1995.
- 14. Natural Products Chemistry Vol 1 and 2, G R Chatwal, Himalaya, New Delhi, 1990
- 15. Comprehensive Organic Chemistry, Vol. 5 (Antibiotics), D. H. R. Barton, W. D. Ollis, Pergamon Press, NY, 1979.
- 16. Organic chemistry Vol.II, I. L. Finar, 6th Edn. Longman, 1992.
- 17. Total synthesis of natural products: The chiral approach Vol.III, S. Hanessian Pergamon Press, 1983.
- 18. Total synthesis of steroids, Akhaun & Titov, Jerusalem, 1969.
- 19. Medicinal natural products: A biosynthetic approach, P. M. Dewick. John Wiley, Chichester, 1997.
- Natural products: Their chemistry and biological significance-J. Mann,
 R. S. Davidson, J. B. Hobbs, D. V. Banthorpe & J. B. Harborne, Longman, UK, 1994.
- Natural products chemistry Vol. I & II, K. Nakanishi, T. Goso, S. Ito, S. Natori & S. Nozoe, Academic Press, NY, 1974.
- 22. Chemistry of natural products Vol. I & II, O. P. Aggarwal, Goel Publishing House, 6th Edn. 1982.
- Total synthesis of natural products: The chiral approach Vol.III, S. Hanessian Pergamon Press, 1983.
- 24. Interpretation of the UV spectra of natural products, A.I. Scott, Pergamon Press, Oxford, 1964.

PRACTICALS

(4 days a week, 4 hours a day)

CH-405 OC: ORGANIC CHEMISTRY PRACTICALS - V

Preparations

- 1. Preparation of NBS from succinic acid and its application in allylic/benzylic brominations
- 2. Photochemical preparation of benzpinacolone from benzophenone.
- 3. Preparation of tetracyclone. Generation of benzyne and its trapping with tetracyclone.
- 4. Synthesis of 2-phenylindole from phenylhydrazone
- 5. Oxidation of anthracene to anthraquinone and conversion to anthrone.
- 6. Reduction of benzoin to stilbene.
- 7. Esterification of 4-nitrobenzoic acid and conversion to benzocaine.
- 8. Preparation of tetraphenyldihydrophthalic anhydride from N-phenylglycine.
- 9. Preparation of 2,4,5-triphenyloxazole from benzoin.
- 10. Biosynthesis of ethanol from sucrose.
- 11. Preparation of methyl red.
- 12. Conversion of 2-naphthol to 1-bromo-2-naphthol.
- 13. Synthesis of hippuric acid.
- 14. Synthesis of 1,2,3,4-Tetrahydrocarbazole.
- 15. Diels-Alder cycloaddition of anthracene with maleic anhydride.
- 16. Synthesis of 2,3-diphenylquinoxaline.
- 17. Green synthesis of acetanilide from aniline.
- 18. Photo-dimerisation of *trans*-cinnamic acide to β -truxinic acid.
- 19. Synthesis of tetraphenylporphyrin.
- 20. Synthesis of Nylon-6,6.

CH-406 OC: ORGANIC CHEMISTRY PRACTICALS - VI

Extractions, Isolations and Separations

Extractions

- 1. Extraction of piperine from pepper.
- 2. Extraction of caffeine from tea leaves.
- 3. Extraction of limonene from citrus fruits rinds'.
- 4. Extraction of azelaic acid from castor oil.
- 5. Extraction of DNA from onion peels.
- 6. Extraction of lycopene from tomatoes.
- 7. Isolation of essential oils from cumin.
- 8. Isolation of essential oils from rose petals.
- 9. Isolation of curcuminoids from turmeric pwoder.

10. Isolation and separation of lactose and casein from milk.

- 11. Isolation and separation of pigments chlorophyll and β -carotene from spinach.
- 12. Separation of caffeine from tannins by sublimation.
- 13. Natural product isolation using steam distillation and liquid phase extraction of thymol, camphor, and citral, monoterpenes sharing a unified biosynthetic precursor

Separations

- 1. Separation of p-rosaniline and methyl red by column chromatography.
- 2. Separation of amino acids by paper chromatography.
- 3. Separation of carbohydrates by thin layer chromatography.
- 4. Separation of *o* and *p*-nitroanilines by thin layer chromatography.
- 5. Separation of anthracene from anthracene picrate.
- 6. TLC of analgesic drugs: acetaminophen, aspirin, caffeine, ibuprofen and salicylamide.

CH-407 OC: ORGANIC CHEMISTRY PRACTICALS - VII

Instrumental methods in organic analysis and quantitative analysis

Instrumental methods in organic analysis

- Recording Recording/predicting/downloading from web sites the UV, IR, NMR and GC-MS/mass spectra of the compounds prepared in C-105/205/305 (Organic Practical – I), C-106/206/306 (Organic Practical – II), C-405 (Organic Practical – III) and C- 406 (Organic Practical – IV).
- 2. Structural elucidation of organic compounds with the help of spectra provided by the instructors/examiners.

Quantitative analysis

Estimations:

- 1. Estimation of Nitro group by reduction using SnCl₂.
- 2. Estimation of Nitrogen by Kjeldahl's method.
- 3. Estimation of an acid in presence of an amide.
- 4. Estimation of an ester in the presence of an acid.

CH-408 OC: ORGANIC CHEMISTRY PRACTICALS - VIII

Quanlitative analysis

Separation of a binary mixture of organic compounds and identification of the separated component/s by systematic qualitative organic analysis.

- 1. Organic Synthesis collective Vols. I to X, 1956-1999. (Freely available on the web)
- 2. Semi-micro qualitative organic analysis, Cheronis, Entrikin & Hoanett.
- 3. Preparation of organic intermediates, D. A. Hirley, John Wiley.
- 4. Text book of practical organic chemistry, A. I. Vogel, Pearson, 5th Edition, Delhi, 2004.

- 5. A laboratory manual of qualitative organic analysis, H.T. Openshaw, Univ. Press, 1999.
- 6. Natural products, Laboratory manual, Ikan, 2000.
- 7. Organic experiments, L. F. Fieser, 2nd Edn. D. C. Heath & Co. USA, 1974-2000.
- 8. Practical organic chemistry F.G. Mann and B. C. Saunders 4th Edn. Longman, 2002.
- 9. Comprehensive practical organic chemistry : Preparation and quantitative Analysis, V. K. Ahluwalia, R. Aggarwal, Universities Press (India), 2000.
- 10. Comprehensive practical organic chemistry: Qualitative analysis, V. K. Ahluwalia, S. Dhingra, Universities Press (India), 2000.
- 11. An advanced course in practical chemistry, A. Ghoshal, B. Mahapatra and A. K. Nad, New central book agency, Calcutta, 2000.
- 12. Advanced practical organic chemistry, J. Mohan, Vol. I and II, Himalaya Publishing House, 1992.
- 13. Practical organic chemistry (Quantitative analysis), B. B. Dey, M V Sitaraman and T. R. Govindachari, Allied Publishers, New Delhi, 1992.
- 14. Laboratory Techniques in Organic Chemistry, V K Ahluwalia, Pooja Bhagat and Renu Aggarwal, I K international Publishing House, New Delhi, 2005.
- 15. Intermediates for Organic Synthesis, V K Ahluwalia, Pooja Bhagat, Ramesh Chandra and Renu Aggarwal, I K international Publishing House, New Delhi, 2005.