Scheme of Study and Examination

I Semester

Course	Title	Hrs/week	Hrs/Semester	Marks	Credit
MCH131	Inorganic Chemistry 1	4	60	100	4
MCH132	Organic Chemistry 1	4	60	100	4
MCH133	Physical Chemistry 1	4	60	100	4
MCH134	Analytical Chemistry	4	60	100	4
MCH151	Inorganic chemistry practicals I	8	120	100	4
MCH152	Physical chemistry practicals I	8	120	100	4

* Mathematics for chemists-30 Hrs. Not intended for ESE.

II Semester

Course	Title	Hrs/week	Hrs/Semester	Marks	Credit
MCH 231	Inorganic Chemistry II	4	60	100	4
MCH 232	Organic Chemistry II	4	60	100	4
MCH 233	Physical Chemistry II	4	60	100	4
MCH 234	Spectroscopy - I	4	60	100	4
MCH 251	Inorganic chemistry practicals II	8	120	100	4
MCH 252	Physical chemistry practicals II	8	120	100	4

* Computer Applications in Chemistry – 30 Hrs. Not intended for ESE.

III Semester

M.Sc. Chemistry (Organic chemistry Specialization)

Course	Title	Hrs/week	Hrs/Semester	Total marks	Credit
MCH 331	Organic reaction mechanisms	4	60	100	4
MCH 332	Organic synthesis- I	4	60	100	4
MCH 333	Chemistry of natural products	4	60	100	4
MCH 334	Spectroscopy – II	4	60	100	4
MCH 351	Organic chemistry practicals - I	8	120	100	4
MCH 352	Organic chemistry practicals - II	8	120	100	4

IV Semester

Course	Title	Hrs/week	Hrs/Semester	Total marks	Credit
MCH 431	Organo-metallic chemistry	4	60	100	4
MCH 432	Stereochemistry & Retro synthetic analysis	4	60	100	4
MCH 433	Organic synthesis II	4	60	100	4
MCH 434	Medicinal organic chemistry	4	60	100	4
MCH 451	Organic chemistry practicals - III	8	120	100	4
MCH 452	Project *			100	4

* The First, Second and Third Semesters of the course involve theory and practicals, while the IV Semester involves theory, practical and project work. The project work shall be carried out for **6 to 8 weeks (at least 30 hrs per week)**, after the Third Semester of the course, either in an institute or in an approved industry or in both, under the supervision of a teacher and submit a project report. Experts from the industries may also be involved in the project work as co-guides and in the evaluation of project reports.

Assessment and Examinations

Continuous internal assessment (CIA) forms 50% and the end semester examination forms the other 50% of the marks in both theory and practical. CIA marks are awarded based on the performance of the students in assignments (written material to be submitted and valued), mid-semester test (MST), and class assignments (Quiz, presentations, problem solving etc.) The mid-semester examination and the end semester examination for each theory paper will be for three hours duration. The CIA for practical sessions is done on a day to day basis depending on their performance in the pre-lab, the conduct of the experiment, and presentation of lab reports. Only those students who qualify with minimum required attendance and CIA will be allowed to appear for the end semester examination.

Examination Pattern for Theory

No.	Component	Schedule	Duration	Marks
CIA1	Mid-Sem Test	[MST]	2 Hrs (50 marks)	25
CIA2a	Assignment/quiz/group task/ presentations	Before MST	--	10
CIA2b	Assignment/quiz/group task/ presentations	After MST	--	10
CIA3	Attendance (75-79 = 1, 80-84 = 2, 85-89 = 3, 90-94 = 4, 95-100 = 5)		--	5
ESE	Centralized		3 Hrs (100 marks)	50
			Total	**100**

End-Semester Exam [ESE]

- A Student is eligible to appear for the ESE only if he has put in 75% of attendance and satisfactory performance in the continuous internal assessment.
- The Question paper shall be set for 100 marks. These marks will then be reduced to 50% of the total marks assigned for the paper.
- There is no provision for taking improvement exams. If a student fails in an ESE paper, he can take the exam again the next time it is offered.
- The Practical examination shall be conducted with one internal and one external examiner. The internal will be the batch teacher, while the external can be from any other institution or another teacher from the same department.
- In the IV Semester there is a project work in lieu of one of the Practicals. The project report shall be evaluated for 75 marks and project related seminar for 25 marks.

Examination pattern for Practical

No.	Component	Duration	Points	Marks
CIA 1	Mid-SemTest [MST]*	4 Hrs	50	20
CIA 2	Class work, Pre Lab assignments	---	40	20
CIA 3	Record book	---	20	10
ESE	(Two examiners)	4 Hrs	50	50
			Total	**100**

Note: Marks will be reduced to 50%

End Semester Practical Examination- Allotment of Marks

Writing Principle, Procedure	:	10
Performing Experiment, Accuracy	:	20
Graph, Calculations, result	:	10
Viva (related to the experiment)	:	10
Total	:	50

Question paper pattern

Question paper has three parts A, B and C. Section A consists of 2 marks questions, section B consists of 5 marks questions and section C consists of 10 marks questions.

- Students have to answer any 10 questions out of 13 in section A, 8 out of 10 in section B and 4 out of 6 in section C.
- Marks from chapters based on the number of teaching hours

Valuation

The valuation will be a centralized one. There will be double valuation of all theory papers (One external and One internal). The average of the marks will be awarded to the candidate.

If the difference in marks is more than 15% the paper will be valued by a third examiner / BOE and the average of the nearest two marks will be awarded to the candidate.

Carry over

For no papers shall the student be allowed to have more than three attempts. He/she should clear the academic arrears within two years after the completion of the course. Note: A student should have passed in at least 50% of the total number of papers of the first year (Semester I and Semester II) to become eligible to get admitted to the third Semester.

Minimum marks requirement

Minimum marks for pass / exemption in each paper is 40%

Minimum marks for pass in the semester is 50% aggregate

There is no separate minimum marks requirement for CIA, however in ESE the candidate should score more than 40% marks in the individual papers and 50% aggregate. If a candidate fails to score 50% aggregate in one or more papers, and 50% aggregate in the semester, he can reappear for ESE in those papers. If a candidate scores more than 40% in all papers and 50% aggregate in the semester he will be declared passed, and will not be eligible for improvement examination.

FIRST SEMESTER

MCH-131 Inorganic Chemistry – I 60 Hrs

1. Chemical Bonding

a. Periodic properties of elements, oxidation numbers, octet rule, concepts of resonance and hybridization. VSEPR model, shapes of molecules; bent rules and energetics of hybridization. Electronegativity and partial ionic character; Bonds: covalent, coordinate, multicentre quadruple and Synergic. Hydrogen bonds – types and detection, agostic bond, Intermolecular forces, metallic bond. **10 Hrs**

b. Lattice energy, Born - Lande equation, Fajans rules, Slater's rules, radius–ratio rules, structures of simple solids and Zintl isoelectric relationships in solids. MO Theory: σ, π and δ molecular orbital, MOs of diatomic molecules, Electron Angular momentum and classification of states**.** **10 Hrs**

2. Chemistry of the main group elements

a. Periodicity and general trends in properties, polymorphism of carbon, phosphorous and sulphur: properties, structure and bonding in boranes, carboranes, borazines, phosphazenes, phosphonitrilic compounds, sulphur–nitrogen compounds, oxyacids of nitrogen, phosphorous, sulphur and halogens; noble gas compounds. **11 Hrs**

b. Silicates–classification and structures, isomorphous replacement, pyroxenes, layered and vitreous silicates, silicate glasses, borosilicate glass ceramics, silica gel, zeolites and molecular sieves, condensed phosphates, polyhalides. **12 Hrs**

c. Solvent systems; Bronsted and Lewis acids and bases, pH and pKa, HSAB concept, acid – base concept in non – aqueous media, leveling effect, super acids, reactions in BF_3, N_2O_4. **7 Hrs**

3. Isopoly and heteropoly acids and their salts. 5Hrs

4. Nuclear chemistry

Sub atomic particles and their properties, nuclear stability, structural models; Liquid drop model and shell model of the nucleus. **5 Hrs**

SUGGESTED BOOKS

1. Basic inorganic chemistry, F.A. Cotton, G. Wilkinson and P.L. Gaus, John Wiley & sons (1995).
2. Advanced inorganic chemistry 6th editions. F.A. Cotton, G. Wilkinson.
3. Inorganic chemistry, 4th edition, J.E. Huheey, E. A. Keiter and R.L. Keiter, Addison – Wesley (1993).
4. Inorganic chemistry, 2nd edition, D.F. Shriver, P.W. Atkins and C.H. Langford, ELBS (Oxford Uni. Press) (1994).
5. Chemistry of the elementals, N.N. Greenwood and A.E. Earnshaw, Butterworth Heinemann (1997).
6. Essential trends in inorganic chemistry, D.M.P Mingos, Oxford Univ. Press (1998).
7. Concise inorganic chemistry; 5th edition; J.D. Lee (1996).
8. Essentials of nuclear chemistry, 4th edition, H.J. Arnikar, NAIL Pub (1995).

MCH 132 Organic Chemistry – I **60 Hrs**

1. Nature of bonding in organic molecules

Delocalized chemical bonding: Conjugation, cross conjugation, resonance, hyper conjugation, bonding in fullerenes. Tautomerism, alternant and non-alternant hydrocarbons. Huckel's rule. Aromaticity in benzenoid and non-benzenoid compounds. Energy level of $\boldsymbol{\pi}$ – molecular orbital, annulenes, antiaromaticity, homo-aromaticity. **7 Hrs**

2. Reaction mechanisms: Structure and Reactivity

Types of mechanisms and reactions. Thermodynamic and kinetic requirements, Hammond's postulate, Curtin-Hammett principle. Potential energy diagrams, transition states and intermediates, methods of determining mechanisms, isotope effects, hard and soft acids and bases.

Generation, structure, stability and reactivity of carbocations, carbanions, carbon free radicals, carbenes and nitrenes.

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

Nucleophilic substitution reaction at a saturated carbon: Limiting cases of SN_1, SN_2 and SN_i mechanisms. Nucleophilicity, leaving group effects, ambident nucleophiles and substrates. **11 Hrs**

3. Stereochemistry

Fischer, Newman, Sawhorse and flying wedge projections and their interconversions. Optical isomerism: Elements of symmetry and chirality. D-L and R-S conventions. Cram's and Prelog's rules. Methods of resolution of optical isomers. Conformational analysis of acyclic compounds: ethane, propane, *n*- butane and 1,2 – disubstituted ethanes. Cyclic alkanes: cyclobutane, cyclohexanes (monomethyl, *iso*-propyl, *tert*-butyl and di- substituted cyclohexanes e.g., dialkyl, dihalo, diols), and cycloheptane. Conformations of fused and bridged ring systems. Prochirality: Enantiotropic and disastereotropic groups and faces.

Geometrical isomerism: *cis – trans* and E-Z conventions. Methods of interconversion of E and Z isomers. **10 Hrs**

4. Natural colouring compounds

Anthocyanins: Methods of isolation, basic structural features of coumarins, chromones, flavones and isoflavones. Structural elucidation and synthesis of quercetin and wedelolactone.

Carotenoids: Methods of isolation. Structural elucidation and synthesis of β-carotene. Structural relationship of α-, β- and γ- carotenes. **8 Hrs**

5. Heterocyclic compounds

Nomenclature of heterocyclic compounds. Structure, reactivity, synthesis and reactions of pyrazole, imidazole, oxazole, isoxazole, thiazole, isothiazole and pyrimidine. Preparation and reactions of quinoline, isoquinoline and indole. **6 Hrs**

6. Carbohydrates

Determination of configuration of the monosaccharide. Conformational analysis of glucose and galactose. Structural elucidation of sucrose and maltose. Synthesis of aldonic, uronic, aldaric acids and alditols. Structures of trehalose, cellobiose, lactose, gentiobiose, meliobiose, starch, cellulose and chitin. Photosynthesis of carbohydrates. **9 Hrs**

7. Vitamins

Biological importance and synthesis of Vitamins A, Vit. B_1 (thiamine), Vit. B_6 (pyridoxine), Vit. C, Vitamin E (α-tocopherol), Vit. H (biotin), Vit. K_1, K_2, folic acid, pantothenic acid and riboflavin. **9 Hrs**

SUGGESTED BOOKS

1. Advanced organic chemistry – Reactions, mechanism and structure, Jerry March, John Wiley, (1999).
2. Advanced organic chemistry, F.A. Carey and R.J. Sundberg Plenum, (1990).

3. A guide book to mechanism in organic chemistry, Peter Sykes, Longman, (2000).
4. Structure and mechanism of organic chemistry, C. K. Ingold, Cornell University Press (1999).
5. Organic chemistry, R T Morrison and R N Boyd, Prentice-Hall, (1998).
6. Modern organic reactions, H O House, Benjamin, (1972).
7. Principles of organic synthesis, R O C Norman and J M Coxon, Blackie Academic and Professional, (1996).
8. Stereochemistry of organic compounds, D Nasipuri, New-Age International, (1999).
9. Stereochemistry of carbon compounds, E L Eliel, S H wilen and L N Mander, John Wiley, (1994).
10. Organic chemistry, Volumes I and II, I L Finar, Longman, (1999).
11. Peptides chemistry : A practical text book, M. Bodansky, Springer-Verlag, NY, (1988).
12. Solid – phase peptide synthesis: A practical approach-E, Artherton & R.C. Sheppard, I R L, Oxford Univ. Press, 1989.
13. Peptides: Chemistry and Biology, N Selwad and H-D. Jakubke, Wiley – VCH, 2002.
14. Natural products chemistry Vol. I &.II, K. Nakanishi, T. Goso, S.Ito, S.Natori & S. Nozoe, Academic Press, NY, 1974.
15. Total synthesis of natural products Vol. I – Vol. VI, Apsimon, John Wiley, NY, 1973 – 1981.

MCH 133 Physical Chemistry – I 60 Hrs

1. Quantum mechanics

a. Equations of wave motion: Progressive and stationery waves, wave equation for a stationary wave (stretched string).

Formulation of quantum mechanics: Wave particle duality of material particles, de Broglie relation, Heisenberg uncertainty principle. Schrödinger wave equation. Time–independent and time-dependent Schrödinger equations and the relations between their solutions. Eigen function and eigen value. Physical interpretation of wave function. Class Q functions. Concept of operators. Laplacian, Hamiltonian, linear and Hermitian operators. Angular momentum operators their properties. Commutation of operators. Normalization, orthogonality and orthonormality of wave functions. Average (expectation) values. Postulates of quantum mechanics. Solutions of Schrödinger equation for a free particle, particle on a ring and particle in a three-dimensional box. Quantum mechanical degeneracy, tunneling (no derivation).

12 Hrs

b. Application of Schrödinger equation to harmonic oscillator and rigid rotator. Eigen functions and eigen values of angular momentum. Ladder operator method for angular momentum. Schrödinger equation to hydrogen atom in spherical polar coordinates. Solution of Φ, θ equations and statement of solution of R equation. Total wave function 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 functions and their significance. Electron spin (Stern – Gerlach experiment), spin orbital, antisymmetry and Pauli's exclusion principle, Slater determinants. Coupling of angular momenta. Russell-Saunders and JJ-coupling, term symbols. Spin-orbit interaction and explanation of term multiplicities (Na-D doublet), Zeeman effect. **12 Hrs**

c. 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 theorem- Statement and proof. Application of variation method to particle in a one dimensional box, linear oscillator and He atom. Slater type orbitals, expressions for Slater orbitals for 1s, 2s, 3s, 2p and 3d electrons (no derivation). Slater's rules for calculation of effective nuclear charge. STOs, for He, C and N. SCF method for many electron atoms. HMO theory for conjugated systems. Application to ethylene, allyl radical, butadiene and benzene. **9 Hrs**

2. Chemical Dynamics

a. Macroscopic and microscopic kinetics**:** Factors affecting reaction rates, Methods of determination of order and rate laws, Collision theory of reaction rates-limitations, Transition state theory. Comparison of collision theory and transition state theory, reaction between ions: influence of ionic strength-primary and secondary kinetic salt effects. Diffusion and activation controlled reactions in solution. **5 Hrs**

b. Steady state kinetics. Chain reactions-general characteristics, chain length and chain inhibition. Mechanisms of thermal reactions (hydrogen-chlorine, phyrolysis of acetaldehyde, decomposition of ethane) and photochemical reactions (H_2 - Br_2 and H_2–Cl_2). Comparative study of thermal and photochemical hydrogen-halogen reactions. **5 Hrs**

c. Theory of homogeneous catalysis, Enzyme catalysis-comparison of enzyme with chemical catalysts, mechanism (lock and key theory), Henri-Michaelis-Menten treatment, significance of Michaelis constant, Lineweaver-Burk plot. Effects of concentration, pH, temperature, activators and inhibitors on enzyme activity. **5 Hrs**

d. Kinetics of fast reactions-study of fast reactions by relaxation method, flow method, flash photolysis and NMR method. Theories of unimolecular reactions, Perrin theory, Lindemann theory, Hinshelwood theory, RRKM theory, Slater treatment. **6 Hrs**

3. Surface Chemistry

Effect of temperature on adsorption, mechanical adsorption, BET and Gibbs adsorption isotherms, estimation of surface area using BET equation, surface tension and surface energy, capillary action, pressure difference across curved surface (Laplace equation), vapour pressure of droplets (Kelvin equation), surface film on liquids (electro-kinetic phenomena), catalytic activity of surfaces. **5 Hrs**

SUGGESTED BOOKS

1. Physical chemistry, P.W. Atkins, Julio de Paula, ELBS, 7th edition, 2002.
2. Physical chemistry: A molecular approach, McQuarie and Simon, Viva, New Delhi, 2001.
3. Introduction to quantum chemistry, A.K. Chandra, Tata McGraw Hill, 1998.
4. Quantum chemistry, Ira N. Levine, Prentice Hall, New Jersey, 1991.
5. Coulson's valence, R.Mc Weeny, ELBS, 1982.
6. Quantum chemistry, 2nd edition, R.K. Prasad, New Age International, 2000.
7. Quantum chemistry, through problems and Solutions, R.K. Prasad, New Age International, 1997.
8. Chemical kinetics – K.J. Laidler, McGraw Hill, Inc. New York, 1988.
9. Principles of chemical kinetics – House J.E. Wm C Brown Publisher, Boston, 1997.
10. Kinetics and mechanism – A.A. Frost and R.G. Pearson, John – Wiley, New York, 1961.
11. Chemical kinetics methods – C.Kalidas, New Age International Publisher, New Delhi, 1995.
12. Kinetics of chemical reactions – S.K.Jain Vishal Publications, Delhi, 1982.
13. Kinetics and mechanism of chemical transformation – J.Rajaraman and J.Kuriakose, Mc Millan, 1986.
14. Physical chemistry of surfaces – A.W. Adamson, Interscience Publisher Inc., New York, 1967.
15. Surface chemistry: Theory and applications, J.J. Bikerman, Academic Press, New York, 1972.

MCH 134 Analytical Chemistry 60 Hrs

1. Role of modern Day Analytical chemistry 3 Hrs

Classifications of analytical methods, types of instrumental analysis, factors influencing choice of analytical method, toxic chemicals sampling and handling hazards, material safety data sheets, miniaturization of analytical methods and its significance in modern chemical analysis.

2. Separation Techniques 22 Hrs

Solvent extraction, efficiency, selectivity, Nernst distribution law, distribution coefficient, derivation for the most efficient extraction, applications and numerical problems. Methods- batch and continuous extraction of liquids, continuous solid-liquid extraction (Soxhlet extraction of phytochemicals) , Craig;s counter current method (not for exam)

Chromatography –classification, mechanisms-adsorption, partition, ion-exchange, gel permeation and affinity chromatography. Performance- retention parameters, theoretical plate, efficiency, resolution, peak broadening- van Deemter equation.

Principles of paper, thin layer, 2D-thin layer chromatography

Gas chromatography-detectors, temperature programming, GC-MS.

Medium performance liquid chromatography, High performance liquid chromatography- theory ,instrumentation and techniques.Normal phase and reversed phase liquid chromatography, Cation and anion exchange chromatography for metals and organic molecules, Gel permeation chromatography for polymers and biomolecules, Super critical liquid chromatography.

Electrophoresis-gel and capillary, mechanism, SDS-PAGE

3. Optical methods of chemical analysis 14 Hrs

Interaction of electromagnetic radiation with matter, Beer-Lambert's law, derivation, verification, deviations, molar extinction coefficient, choice of solvent, Sandell sensitivity, Ringbom's plot, photometric titrations, Single beam and double beam UV-VIS spectrophotometer, Atomic absorption spectroscopy- instrumentation and application in quantitative and qualitative analysis, Numerical problems.

Principle, instrumentation and applications of fluorimetry, turbidimetry and nephelometry, ORD and CD.

4. Electro analytical methods. 10hrs

Potentiometry- electrode systems, potentiometric titrations- acid- base, precipitation and redox titrations.

Polarography and Voltammetry- Diffusion currents, half-wave potentials, characteristics of the DME, Amperometric titrations, applications of polarography and amperometric titrations.

Electrogravimetry, Coulometry, Coulometry at constant potential, coulometric titrations, applications.

Conductometric titrations- ionic conductances, acid-base titrations.

5. Thermal methods of analysis. 4Hrs

Theory, instrumentation and applications of TGA, DTA and DSC.

6. Radio analytical methods 7Hrs

Radioactivity, ionization, working principles of scintillation counter, GM counter, semiconductor counter. Radio analytical methods- neutron activation analysis, isotopic dilution analysis, radiotracer technique. Applications of all these techniques, use of radioactive isotopes in solving analytical and physico chemical problems.

SUGGESTED BOOKS

1. Analytical chemistry G.D. Christian, V edition, John – Wiley and Sons Inc., 1994.
2. Instrumental methods of analysis H.H. Willard, L.L. Merrit, J.A. Dean and F.A. Set, CBS Publishers, 1996.
3. Electrochemical methods: A.J. Bard & I.R. Faulkner, 2nd edition, Wiley, New York, 2000.
4. Principles and techniques of Biochemistry and Molecular biology, VIth Edition, Keith Wilson and John Walker.

5. Fundamentals of analytical chemistry, 8th edition, Skoog, West, Holler and Crouch: Thomson Asia Pvt. Ltd, 2004.
6. Principles and practice of Analytical Chemistry, Vth edition F.W.Fifield and D. Kealy.

Mathematics for Chemists- 30Hrs

I Vectors and Matrix Algebra — 10 Hrs

A Vectors

Vectors, dot, cross and triple products etc. The gradient, divergence and curl. Vector calculus, Gauss' theorem, divergence theorem etc.

B. Matrix Algebra

Addition and multiplication; inverse, adjoint and transpose of matrices, special matrices (Symmetric, skew-symmetric, Hermitian, skew-Hermitian, unit, diagonal, unitary etc.) and their properties. Matrix equations: Homogeneous, non-homogeneous linear equations and conditions for the solution, linear dependence and independence.

Introduction to vector spaces, matrix eigenvalues and eigenvectors, diagonalization, determinants (examples from Hückel theory).

Introduction to tensors; polarizability and magnetic susceptibility as examples.

II Differential Calculus — 10 Hrs

Functions, continuity and differentiability, rules for differentiation, applications of differential calculus including maxima and minima (examples related to maximally populated rotational energy levels, Bohr's radius and most probable velocity from Maxwell's distribution etc), exact and inexact differentials with their applications to thermodynamic properties.

Integral calculus, basic rules for integration, integration by parts, partial fraction and substitution. Reduction formulae, applications of integral calculus.

Functions of several variables, partial differentiation, co-ordinate transformations (e.g. cartesian to spherical polar), curve sketching.

III Elementary Differential Equations — 7 Hrs

Variables-separable and exact first-order differential equations, homogeneous, exact and linear equations. Applications to chemical kinetics, secular equilibria, quantum chemistry etc. Solutions of differential equations by the power series method, Fourier series, solutions of harmonic oscillator and Legendre equation etc., spherical harmonics, second order differential equations and their solutions.

IV Permutation and Probability 3 Hrs

Permutations and combinations, probability and probability theorems, probability curves, average, root mean square and most probable errors, examples from the kinetic theory of gases etc., curve fitting (including least squares fit etc.) with a general polynomial fit.

Books Suggested

1. The Chemistry Mathematics Book, E. Steiner, Oxford University Press.
2. Mathematics for Chemistry, Doggett and Sutcliffe, Longman.
3. Mathematical Preparation for Physical Chemistry, F. Daniels, McGraw Hill.
4. Chemical Mathematics, D.M. Hirst, Longman.
5. Applied Mathematics for Physical Chemistry, J.R. Barrante, Prentice Hall.
6. Basic Mathematics for Chemists, Tebbutt, Wiley.

MCH 151 AND MCH 152: PRACTICALS

(4 days a week, 4 hours a day)

MCH 151 Inorganic chemistry practical - I

A. **Semi-micro qualitative analysis** of mixtures containing two each of common cations and anions and one of the following less familiar elements: W, Se, Mo, Ce, Th, Zr, V, U and Li.

B. Preparation and quantitative analysis of inorganic complexes

1. Ferrous oxalate
2. Potassium trioxalatofetrrate (III) trihydrate.
3. Hexammine cobalt (III) chloride.
4. Cis and trans-potassium dioxalatodiaquochromium (III).

SUGGESTED BOOKS

1. Vogel's text book of qualitative chemical analysis, J. Bassett, G.H. Jeffery and J.Mendham, ELBS, 1986.
2. Vogel's text book of qualitative chemical analysis, 5th edition, J. Bassett, G.H. Jeffery and J.Mendham, and R.C. Denny, Longman Scientific and Technical, 1999.
3. Inorganic semi micro qualitative analysis, V.V. Ramanujam, The National Pub. Co., 1972.
4. Practical inorganic chemistry, G.Marr and B.W. Rockett, Von Nostrand Reinhold, 1972.

MCH 152 Physical Chemistry Practical – I

Chemical Kinetics

1. Determination of the velocity constant, catalytic coefficient, temperature coefficient, $t_{1/2}$ and energy of activation for the acid hydrolysis of methyl acetate.
2. Evaluation of Arrehenium parameters for the reaction between potassium persulphate and potassium iodide (1^{st} order).
3. Velocity constant for the saponification of ethyl acetate.
4. Determination of the order of reaction between hydrogen peroxide and potassium iodide (clock reaction).

Colorimetry

5. Test for the validity of Beer–Lambert Law and determination of the unknown concentration of a solution. Calculation of molar extinction coefficient.
6. Titration of ferrous ammonium sulfate with potassium permanganate colorimetrically.
7. Simultaneous estimation of Mn and Cr in a solution of $KMnO_4$ and $K_2Cr_2O_7$.
8. Kinetics of reaction between $K_2S_2O_8$ – KI Colorimetrically.
9. Determination of concentration of Fe by spectrophotometric titration using EDTA.

Cryoscopy

10. Determination of molecular weight of a solute by cryoscopy.
11. Determination of degree of dissociation of an electrolyte and association of benzoic acid in benzene.

Partial Molal Volume

12. Determination of partial molal volume of ethanol by reciprocal density method.
13. Determination of PMV by apparent molar volume method, NaCI – H_2O system.

Phase diagram

14. Construction of phase diagram of a two–component system and determination of eutectic temperature and eutectic composition.

Adsorption

15. Adsorption of oxalic on charcoal. Verification of Langmuir adsorption isotherm.

SUGGESTED BOOKS

1. Findlay's practical physical chemistry revised by Levitt, Longman's London, 1966.
2. Experiments in physical chemistry by Shoemaker and Garland, McGraw Hill International edn., 1996.
3. Advanced practical chemistry by J.B. Yadav, Goel Publication house, Meerut, 1989.
4. Experimental physical chemistry by Daniel etal., McGraw Hill, 1962.
5. Experimental physical chemistry by Wilson, Newcombe and others, Pergamon Press, New York, 1962.
6. Practical physical chemistry by A.M. James and D.E. Pritchard, Longman Group Ltd.1968.
7. Experimental physical chemistry, V.D. Athawale and Parul mathur, New Age International, New Delhi, 2001.
8. Experiments in physical chemistry, J.G. Ghosh, Bharathi Bhavan, 1974.

SECOND SEMESTER

MCH 231: Inorganic Chemistry – II (Co-Ordination Chemistry) 60 Hrs

1. 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 and macrocylic effects and their thermodynamic origin, determination of binary formation constants by pH-metry, spectrophotometry, polarography and by ion exchange methods. **12 Hrs**

2. Metal – Ligand bonding

Crystal field theory-limitation, stereochemistry, coordination Nos, 3 to 8, evidences for metal–ligand orbital overlap, MO theory (including π-bonding), Jahn–Teller distortion in metal complexes and metal chelates, spectrochemical series, nephelauxetic series, angular overlap model. **10 Hrs**

3. Structure and bonding

Hydride, dihydrogen, simple metal carbonyl, nitrosyl, dinitrogen and tertiary phosphine complexes, metal complexes as liquid crystals, stereo chemical non-rigidity, self-assembly in supramolecular chemistry; stereoisomerism-chirality, optical activity, CD, ORD, cotton effect and magnetic circular dichrosim, absolute configurations. **16 Hrs**

4. Electronic spectra of transition metal complexes

Spectroscopic ground states, selection rules, term symbols for d^n ions, Racah parameters, Orgel correlation and Tanabe-Sugano diagrams, spectra of 3d metal aqua

complexes of trivalent V, Cr, divalent Mn, Co and Ni, $[CoCI_4]^{2-}$, calculation of Dq, B and β parameters, charge transfer spectra. **14 Hrs**

5. Magnetic properties of metal complexes

Magnetic susceptibility, types of magnetic behaviour, diamagnetic corrections, orbital contribution, spin-orbit coupling, Ferro and antiferromagnetic coupling, spin crossover. **6 Hrs**

SUGGESTED BOOKS

1. Basic inorganic chemistry, F.A. Cotton, G. Wilkinson and P.L. Gaus. John Wiley & sons Inc, 6th edition, 1999.
2. Inorganic chemistry, 4th edition, J.E. Huheey, E.A. Keiter and R.L. Keiter, Addison-Welsey, 1993.
3. Inorganic chemistry, 2nd edition, D.F. Shriver, P.W. Atkins and C.H. Langford, ELBS (Oxford Uni. Press), 1994.
4. Chemistry of the elementals, N.N. Greenwood and A.E. Earnshaw, Butterworth Heinemann, 1997.
5. Inorganic electronic spectroscopy, A.B.P. Lever, Elsevier.
6. Essential trends in inorganic chemistry, D.M.P. Mingos, Oxford Univ. Press, 1998.
7. Magnetochemistry, R.L. Carlin, Springer Verlag.
8. Electronic absorption spectroscopy and related techniques, D.N. Sathyanarayana, Universities Press, 2001.

MCH 232 Organic Chemistry – II **60 Hrs**

1. Aromatic substitution reactions

Electrophilic substitution reactions : 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. Diazonium coupling, Vilsmeir reaction, Gattermann-Koch reaction.

Nucleophilic substitution reactions: The SN Ar, SN1, benzyne and SRN1 mechanisms. Reactivity – effect of substrate structure, leaving group and attacking nucleophile. The von Richter, Sommelet-Hauser and Smiles rearrangements. **10 Hrs**

2. Addition reactions

Addition to carbon multiple bonds: Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals. Regio, stereo and chemoselectivities. Orientation and reactivity. Addition to cyclopropane ring. Hydrogenation of double and triple bonds, hydrogenation of aromatic rings. Hydroboration, Michael reaction

Addition to carbon-heteroatom multiple bonds: Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acids, esters and nitriles. Additional of Grignard reagents and organolithium reagents to carbonyl compounds and unsaturated carbonyl compounds. Addition of water and formation of acetals, ketals, oximes and hydrazones from carbonyl compounds, Wittig reaction. Mechanism of condensation reactions involving enolates-Aldol, knoevenagel, Clasisen, Mannich, Benzoin, Perkin and Stobbe reactions. Ammonolysis of esters, hydrolysis amides. **13 Hrs**

3. Elimination reactions

The E2, E1 and E1cB mechanisms and their spectrum. Orientation of the double bond. Reactivity – effects of substrate structure, attacking base, the leaving group and the medium. Mechanism and orientation in pyrolytic elimination. **5Hrs**

4. Rearrangements

Wagner–Meerwein, Pinacol–Pinacolone, Fries, Wolff, Beckmann, Hofmann, Curtius Lossen and Schmidt rearrangements. **6Hrs**

5. Nucleic acids

Introduction, protecting groups for hydroxyl group in sugar, amino group in the base and phosphate functions. Methods of formation of internucleotide bonds: DCC, phosphodiester and phosphodiester approaches, phosphate triester and phosphoramide methods. Solid phase synthesis of oligonucleotides. **7 Hrs**

6. Peptides

Classification and nomenclature. 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, acid halides, anhydrides in peptide bond formation reactions. Deprotection and racemization in peptide synthesis. Solution and solid phase techniques. Synthesis of oxytocin, gramicidin, enkephalins, LH-RH. Introduction to peptidomimetics. **12 Hrs**

7. Synthetic molecular receptors

Definition and significance. Structures and function of receptors with molecular clefts. Molecular tweezers, macro cyclic polyethers, receptors with multiple hydrogen bonding sites, cyclophanes, calixarenes and cyclodextrins. **7 Hrs**

SUGGESTED BOOKS

1. Advanced organic chemistry – Reactions, mechanism and structure, Jerry March, John Wiley, 1999.

2. Advanced organic chemistry, F.A. Carey and R.J. Sundberg, Plenum, 1990.
3. A guide book of mechanism of organic chemistry, Peter Sykes, Longman, 2000.
4. Structure and mechanism of organic chemistry, C.K. Ingold, Cornell University Press.
5. Organic chemistry, R.T. Morrison and R.N. Boyd, Prentice-Hall, 1998.
6. Modern organic reactions, H.O. House, Benjamin, 1972.
7. Principles of organic synthesis, ROC Norman and J.M. Coxon, Blackie Academic and Professional, 1996.
8. Stereochemistry of organic compounds, D. Nasipuri, New-Age International, 1999.
9. Stereochemistry of carbon compounds, E.L. Eliel, S.H. Wilen and L.N. Mander, John Wiley, 1994.
10. Organic chemistry, Volumes I and II, IL Finar, Longman, 1999.
11. Medicinal chemistry, A Kar, Wiley, 2000.
12. Peptides chemistry: A practical text book, M. Bodanzsky, Springer – Verlag, NY, 1988.
13. Solid-phase peptide synthesis: A practical approach-E, Artherton & R.C. Sheppard, I R L, Oxford Univ. Press, 1989.
14. Peptides: Chemistry and biology, N Selwad and H.D. Jakubke, Wiley – VCH, 2002.

MCH 233 Physical Chemistry – II 60 Hrs

1. Thermodynamics

a. **Classical thermodynamics:** Brief resume of concepts of laws of thermodynamics – free energy, chemical potential and entropies. Partial molar properties – partial molar free energy, partial molar volume, partial molar heat content and their significance. Determination of these quantities. Concept of fugacity and its determination by graphical method and compressibility factor method. Non ideal systems–Excess functions for non-ideal solutions. Activity and activity coefficient. Relationship between mole fraction, molality and molarity activity coefficients. Determination of activity coefficient by EMF and solubility methods. Phase rule – Derivation of phase rule from the concept of chemical potential, application of phase rule to three component systems. **11 Hrs**

b. **Statistical thermodynamics:** Concepts of distribution, thermodynamic probability and most probable distribution. Ensemble averaging–postulates of ensemble averaging. Canonical, grand canonical and micro canonical ensembles with corresponding distribution laws (using languages method of undetermined multipliers). Partition functions – translational, rotational, vibrational and electronic partition functions. Calculation of thermodynamic properities in terms of partition functions. Applications of partition functions. Fermi-Dirac statistics – distribution law and applications to metal. Bose-Einstein statistics-distribution law and application to helium. Heat capacity behavior of solids. **12 Hrs**

c. **Non equilibrium thermodynamics:** Thermodynamic criteria for non-equilibrium states, entropy production and entropy flow. Entropy balance equation for different

irreversible processes (e.g., heat flow, chemical reaction etc.). Transformations of the generalized fluxes and forces, non equilibrium stationary states, phenomenological equations, microscopic reversibility and Onsager's reciprocity relations. **6 Hrs**

2. Electrochemistry

a. **Electrochemistry of solutions:** Ionic atmosphere, physical significance of K (Cuppa), Debye-Huckel theory to the problem of activity coefficient, Debye Huckel limiting law, Debye Huckel equation for appreciable concentration, the Huckel and Bronsted equation, qualitative verification of Debye-Huckel equation, Debye-Huckel Onsagar conductance equation, Bjerrum theory of ion association-triples ion-conductance minima. **12 Hrs**

b. **Electrical double layer:** Introduction to electrode – electrolyte interface. Diffuse double layer, Stern Theory of double layer, thermodynamics of electrified interfaces, concept of surface excess, thermodynamics of surface excess, determination of charge density on the electrode. Derivation of electro capillary–Lipmann equation. **9 Hrs**

c. **Irreversible electrode process:** Irreversible electrode process: polarization and over voltage, types of overvoltages. Electrolytic polarization, dissolution and deposition potential. Determination of anode and cathode overpotential, concentration polarization, Variation of current with cell voltage, metal deposition overvoltage, Thickness of the diffusion layer, Derivation of Butler- volmer equation, Exchange current density factors affection exchange current density. Influence of current density, pH, temperature, rate of growth of deposits on over voltage.

Theories of overvoltage: Bubble formation, Combination of atoms, Ion discharge and proton transfer as slow process. **10 Hrs**

SUGGESTED BOOKS

1. Kinetics and mechanism of chemical transformation, J, Rajaraman and J. Kuriacose, Mc Millan, (1986)
2. Molecular thermodynamics, Donald A. Mc Quarrie, John D.Simon University Seience Books, California, (1999)
3. Thermodynamics for Chemists by S. Glasstone, Affiliated East- west Press Ncw Delhi, (1960)
4. Thermodynamic Rajaraman and Kuriacose, East West, 1986.
5. Statistical Thermodynamics, M.C Gupta (Wiley eastern Ltd.) 1993.
6. Elementary Statistical Thermodynamics, N. D Smith, Plenum press, N.Y. (1982).
7. Elements of Classical and Statistical Thermodynamics, L.K. Nash, Addison-Wiley (1970).
8. Modern Electrochemistry- Vol. I and II, J.O. M. Bockris and A.K.N. Reddy, Plenum, New York (1978).
9. An Introduction to Electrochemistry-Samuel Glastone, East-West edition, New Delhi(1942).
10. Text Book of Physical Chemistry- Samuel Glastone, 2nd edition, Mc Millan India Ltd. (1991).
12. Principles and Applications of Electrochemistry- D.R. Crow, 3rd ed., (Chapman hall, London)1988.

MCH 234 Spectroscopy-I **60 Hrs**

1. **Symmetry and Group Theory in Chemistry**

   Definitions of group, subgroup cyclic groups, conjugate relationships, classes, simple theorems in group theory. Symmetry elements and symmetry operations, point groups, Schöenflies notations, representations of group by matrices, reducible and irreducible representations, characters of representations, Great Orthogonality Theorem (without proof) and its applications, character tables and their uses (representation for the Cn, Cnv, Cnh, Dnh 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. **14 Hrs**

2. **Unifying principles**

   Interaction of electromagnetic radiation with matter- time dependent perturbation theory, transition moment integral, and selection rules-symmetry and spin forbidden transitions. **3 Hrs**

3. **Microwave Spectroscopy**

   Rotations of molecules, rigid diatomic molecule- rotational energy expression energy level diagram, rotational wave function 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. **7 Hrs**

4. Infrared Spectroscopy

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 line, computation of intensities, hot bands, effect of isotopic substitution.

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

Vibrations of polyatomic molecules: Normal coordinates,trans1ations, vibrations and rotations, vibrational energy levels and wave functions, fundamentals, overtones and combinations.

Vibration-rotation spectra of polyatomic molecules- parallel-and perpendicular vibrations of linear and symmetric top molecules. Techniques and instrumentation, FTIR . **14 Hrs**

5. 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 polarization of Raman scattered photons.

Structure determination from Raman and IR spectroscopy-AB_2 and AB_3 molecules Techniques and instrumentation. **8 Hrs**

6. 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 resu1ts MO theory, classification of states by electronic angular momentum-Σ, Δ Π and Φ 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. **14 Hrs**

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. Student Edition)(1990)
6. Spectroscopy, Vols 1-3 B.P. Straughan W. Walker, Chapman Hall (1976) Modern Spectroscopy, J.M. Hollas, John Wiley.

Computers for Chemists- 30Hrs

I. Microsoft Office

Microsoft Word **3 Hrs**

Working with text, Working with Paragraphs, Working with Documents, Using Tables, Working with Pictures and Charts, Using Mail Merge

Ms-Excel **5 Hrs**

Getting Started with Excel, Building and Editing Worksheets, Formatting a Worksheet, Working with Charts, Working with Formulas and Functions, Automating Worksheet Tasks with Macros, Using Lists, Analyzing List Data, Enhancing Charts and Worksheets, Using Analysis Tools, Analyzing Data with Pivot Tables, Programming using Excel Macros.

Microsoft PowerPoint **2 Hrs**

Creating a Presentation, Modifying a Presentation, Working with Text, Working with Visual Elements , Customizing a Presentation , Creating Output , Delivering a Presentation , Managing Files

II . Use of Computer Programmes **20 Hrs**

The students will learn standard programs and packages such as MS-WORD, EXCEL, ORIGIN, SIGMA PLOT, CHEM SKETCH etc. and solve chemistry problems taken preferably from physical chemistry for plotting first and second derivative curves, linear plots etc. Solving problems from chemical kinetics, polymer chemistry, analytical chemistry, electrochemistry, spectroscopy etc. Practice of writing the structures of

inorganic and organic molecules, writing chemical equations, determining molecular parameters such as bond lengths, bond angles, dihedral angles etc.

Introduction to chemistry based web packages on the internet depending on the availability.

Reference Books

1. Computers and their applications to Chemistry, Ramesh Kumari, Narosa

2.Theory and Problems of Programming with Basic, Mc graw Hill, NY,1987.

3.Programming with Fortran 77, Ram Kumar, Tata McGraw Hill, 1989.

4.Fortran 77 with Applications to Science & Engg -Jain & Suri,Tata McGraw Hill, 1982.

5.Computer programming in Fortran IV,V , Rajaraman, Prentice Hall of India, 1987.

6.Computers in Chemistry & Instrumentation,Vol.1-5 Mattson, Marcel Dekker, NY,1974

7.Numerical methods in chemistry. , K. J. Johnson, Marcel Dekker , NY, 1980.

8.Computers in Chemistry, K. V. Raman , TMH, 1993.

Note: The remaining hours could be utilized for lab and additional hours given if needed.

MCH 251 AND MCH 252: PRACTICALS

(4 Hrs per day, 4 days per week)

Experiments are as in first semester. Every student will carry out experiments in each of the two branches of chemistry on a rotation basis.

MCH 251 Inorganic Chemistry Practical – II

1. Gravimetric determination of Fe in an iron ore as Fe_2O_3.
2. Volumetric/redox and gravimetric determination of the following mixtures: (a) Copper and nickel (b) Copper and iron (C) Copper and Zinc (d) Nickel and zinc (e) Iron and chromium.
3. Analysis of alloys: (a) German silver (b) Steel (c) Solder.
4. Analysis of ores: (a) Haematite, (b) Dolomite, (c) Pyrolusite
5. Flame photometric determination of Na/K in cement and soil samples.

SUGGESTED BOOKS

1. Text Book of Quantitative Inorganic Analysis by A.I. Vogel, ELBS (1978).
2. Advanced Physicochemical Experiments by Rose, Issac Pitman (1964)
3. Polarographic methods of analysis by Meites, L. Intersciences, Publishers, Inc. New York, (1955).
4. Findlay's Practical Physical Chemistry by Levitt, Longmann's (1966)
5. Experimental Physical Chemistry by Wilson, Newcombe, Denaro and Rickett, Pergamon Press, (1962).
6. Practical Physical Chemistry by Palit and De, Science Book Agency, Calcutta, (1974).
7. Advanced Physical Chemistry by J.B. Yadav, Goel Pub, House, (1981)

8. Methods of Soil Analysis Part I & II, C.A. Black et al (Ed) American Society of Agronomy, Inc., (1965).

MCH 252 Physical Chemistry Practical – II

Conductivity

1. Determination of the solubility of a sparingly soluble salt.
2. Titration of mixture of strong and weak acids against a strong base.
3. Titration of mixture of strong acid, weak acid and salt (copper sulfate) against strong base.
4. Titration of weak acid against a weak base.
5. Precipitation titration: Lithium sulfate against barium chloride.
6. Dissociation constant of weak electrolyte (weak base – NH_4OH; weak acid – CH_3COOH).
7. Verification of Onsager's equation – determination of λ_0 of an electrolyte.

Potentiometry

1. Determination of single electrode potential of Cu^{2+} / Cu and Zn^{2+} / Zn and testing the validity of Nernst equation.
2. Determination of pH of buffers by using quinhydrone electrode and comparison of the pH values obtained with glass electrode.
3. Potentiometric titration of ferrous ammonium sulfate against potassium dichromate – calculation of formal redox potential of Fe^{3+} / Fe^{2+} .
4. Potentiometric titration of potassium iodide against potassium permanganate.
5. Titration of silver nitrate against potassium chloride.
6. Determination of EMF of a concentration cell and calculation of solubility product of AgCl.

7. Titration of weak acid against a strong base using quinhydrone electrode and calculation of pK_a value of the weak acid.
8. Titration of a mixture of HCI and CH_3COOH potentiometrically and determination of the composition of the mixture.

SUGGESTED BOOKS

1. Findlay's practical physical chemistry revised by Levitt, Longman's London, 1966.
2. Experiments in physical chemistry by Shoemaker and Garland, McGraw Hill International edn., 1996.
3. Advanced practical chemistry by J.B. Yadav, Goel Publication house, Meerut, 1989.
4. Experimental physical chemistry by Daniel etal., McGraw Hill, 1962.
5. Experimental physical chemistry by Wilson, Newcombe and others, Pergamon Press, New York, 1962.
6. Practical physical chemistry by A.M. James and D.E. Pritchard, Longman Group Ltd.1968.
7. Experimental physical chemistry, V.D. Athawale and Parul mathur, New Age International, New Delhi, 2001.
8. Experiments in physical chemistry, J.G. Ghosh, Bharathi Bhavan, 1974.

THIRD SEMESTER

MCH 331 Organic Reaction Mechanisms 60 Hrs

1. **Aliphatic nucleophilic and electrophilic substitution**

Nucleophilic substitution reactions: Substitution at allylic and trigonal carbon atoms. Hydrolysis of esters, use DCC in the formation of anhydrides. Neighbouring group participation.

Electrophilic substitution reactions: SE_2, SE_1 and SE*i* mechanisms. Hydrogen exchange, migration of double bonds, halogenation of aldehydes, ketones and acids. Aliphatic diazonium coupling, nitrosation at carbon and nitrogen, diazo transfer reaction, carbine and nitrene insertion, decarboxylation of aliphatic acids, haloform reaction, Haller-Bauer reaction. **12 Hrs**

2. **Free-radical chemistry**

Generation of free radicals: Thermal homolysis of per esters and azo compounds, photochcmical methods. Hydrogen abstraction, chain process.

Stability: Steric, resonance and hypercojugative effects. Structure and stereochemistry of free radicals. Free radical reactions: Addition, elimination, rearrangement and electron transfer reactions. Use of free radicals in organic synthesis. **8 Hrs**

3. **Photochemistry**

General consideration: Activation in thermal photochemistry reactions. Light absorption and excitation. Phosphorescence and fluorescence, Singlet and triplet states. Morse curve, Franck-Condon principle.

Excitation: Physical process, in thermal and photosensitization (donor acceptor concept, resonance and collision transfer). Chemical process, quantum efficiency, quantum and chemical yields.

Photochemistry of functions group

a. Olefins: Cis-trans isomerism, [2+2] cycloaddition, rearrangements, Reaction of conjugated olefins: di-π -methane rearrangement.
b. Ketones: Excited state of C=O, Norrish type-I and type-II cleavages, Paterno- Buchi reaction, α,β-unsaturated ketones, [2+2] addition, cis-trans isomerisation, Rearrangements of cyclohexadienones.
c. Aromatic compounds: Photorearrangement of benzene and its derivatives and cycloaddition of benzene.
d. Photochemical oxidations and reductions: Cycloaddition of singlet molecular oxygen. Oxidative coupling of aromatic compounds and photoreduction by hydrogen absorptions. **14 Hrs**

4. Pericyclic reactions

Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3 butadiene, 1,3,5-hexatriene and allyl system. Classification of pericyclic reactions. Woodward-Hoffmann correlation diagrams. FMO and PMO approach. Electrocyclic reactions – conrotatory and disrotatory motions: 4n, 4n+2 and allyl systems. Cycloaddition – antarafacial and suprafacial additions, [2+2] additions of ketenes, 1,3-dipolar cycloadditions and cheleotropic reactions.

Sigmatropic rearrangements- suprafacial and antarafacial shifts of H, sigmatropic shifts involving carbon moieties. [3,3]- and [5,5]- sigmatropic rearrangement, Claisen, Cope and aza-Cope rearrangements. **14 Hrs**

5. Biochemical mechanisms

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

a. Thiamine pyrophosphate (TPP) in decarboxylation of α-ketoacids and in the formation of α-ketols.
b. Pyridoxal phosphate (PLP) in transamination, decarboxylation, dealdolisation and elimination reactions of amino acids.
c. Lipoic acid in the transfer of acyl group reactions.

d. Coenzyme A (CoASH) in the transfer of acyl group.
e. Biotin in the carboxylation reactions.
f. Tetrahydrofolic acid (H4F) in one –carbon transfer reactions.
g. Vitamin B_{12} coenzymes in molecular rearrangement reactions and in the synthesis of methionine and methane.
h. Nicotinamide and flavin coenzymes in biological redox reactions. **12 Hrs**

SUGGESTED BOOKS

1. Understanding organic reaction mechanisms, A. Jacob, . Cambridge Univ Press 1997
2. Introduction to organic chemistry A. Streitweiser, Jr and C.H Heathcock Macmillan, 1985
3. Physical and mechanistic organic chemistry, R.A.Y. Jones, 1st Edn. Cambridge univ Press 1979.
4. Mechanisms of molecular migrations, Vols I and II B.S. Thiagarajan, 1st Edn. Pergamon Press, Oxford,1979.
5. P.J. Garratt in Comprehensive organic chemistry, D. Barton and W.D. Ollis, 1st Edn. Pergamon Press, Oxford, 1979.
6. Radicals in organic synthesis, B Giese, Pergamon Press, 1986.
7. Stereo electronic effects in organic chemistry, P.Deslongchamps, 1st Edn,

MCH 332 Organic Synthesis I **60Hrs**

1. **C-C and C-N bond forming reactions**

   Friedel-Crafts reaction, Diels-Alder reaction, Chichibabin reaction, Darzen's reaction, Use of acetylides in C-C bond formation reaction. Acid-catalyzed self condensation of olefins, Skraup synthesis, Prins reaction, Shapiro reaction, Dieckmann cyclisation, Reformatsky reaction, Robinson annelation, Hofmann- Loeffler- Freytag reaction.

   Stork–enamine synthesis. Meyer synthesis. Use of nucleophilic nitrogen and electrophilic carbon (NH_3 amines and nitrite as nucleophiles in substitution, NH_3 and amines in addition to ketones and aldehydes) and electrophilic nitrogen and nucleophilic carbon (nitration) in the bond formation reactions. **15 Hrs**

2. **Reagents in organic synthesis**

   Use of the following in organic synthesis and functional group tansformations. LDA, DCC, DDQ, TMS-iodide, TMS- cyanide, TBDMS-Chloride, 1,3-Dithiane (reactivtity and umpolung), Merrifield resin, Baker's yeast. Woodward and Prevost hydroxylation, Peterson reaction. **11 Hrs**

3. **Oxidations**

   CrO_3, $K_2Cr_2O_7$, $KMnO_4$, OsO_4, SeO_2, $Pb(OAc)_4$, HIO_4 oxygen (singlet & triplet), ozone, Peroxides and Peracids as oxidizing agents. Oppenauer oxidation. **11 Hrs**

4. **Reduction**

   Complex metal hydrides, dissolving metal reductions diimide reduction, catalytic hydrogenation (homogeneous and heterogeneous) tri-n-butyltin hydride and

organoboranes as reducing agents. Meerwein-Ponndorf-Verley, Wolf- Kishner and Clemmensen reductions. **11 Hrs**

5. Molecular rearrangements

Benzil-benzilic acid rearrangement, Arndt- Eistert reaction, Tiffeneau- Demjanov reaction, Firtsch-buttenberg-Wiechell rearrangement. Stevens, Wittig Favorskii and Fries rearrangements. Baeyer-Villiger oxidation. Neber rearrangement, and rearrangement of amino ketones. Mechanism of Fischer indole synthesis and benzidine rearrangement. **12 Hrs**

SUGGESTED BOOKS

1. Advanced organic chemistry, J. March, 5th Edn. John Wiley,1999.
2. Organic synthesis R.E .Ireland, Prentice-hall India, New Delhi, 1975.
3. Understanding organic reaction mechanisms, QA, Jacob Cambridge Univ Press1997
4. Introduction to organic chemistry, A. streitwesiser, Jr and C.H Heathcock,Macmillan,1985.
5 Physical and mechanistic organic chemistry, R.A.Y. Jones, 1st Edn. Cambridge Univ Press, 1979.
6. Modern synthetic reactions, H.O. House, W.A. Benjamin, California, 2nd Edn. 1972.
7. Some modern methods of organic synthesis, W Carruthurs, Cambridge Univ. Perrganmon Press, London, 2nd Edn. 1979.
8. Mechanisms of molecular migration, Vols I& II B.S. Thyagarajan.Pergamon Press, Oxford, 1979.
9. Comperhensive organic chemistry, D. barton and W.D. Wallis Pergamon Press Oxford, 1983.
10. Organic chemistry Vol. II I.L Finar 6th Edn. Longman 1992.

MCH 333 Chemistry of Natural Products 60Hrs

(NOTE : For structural elucidation, emphasis is to be placed on the use of spectral parameters wherever possible)

1. Terpenoids

Classification, nomenclature, occurrence and isolation. Isoprene rules. Stereochemistry of citral, farnesol, limonene, 1,8-cineole, menthols and borneols. Correlation of configuration of terpenoids. Structure elucidation of α-pinene, camphene, β- caryophyllene, α- santonin and gibberrillic acid.

Synthesis and biosynthesis of the following: Linalcol, α-terpineol, fenchone, eudesmol and abietic acid.

Commercial synthesis of camphor. Biosynthesis of squalene and cyclisation of squalene into α-lanosterol and friedelene. **13 Hrs**

2. Steroids

Occurrence. Nomenclature, basic skeleton, Diels hydrocarbon and stereochemistry. Isolation, structure and structural elucidation of sterols and bil acids. Sex hormones and corticosteroids. Synthesis of cholesterol, estrone, progesterone, epiandrosterone and testosterone. Photo products of ergosterol- vitamin D. Barton reaction for the synthesis of aldosterone.

Marker degradation. Brief discussion of homosteroids, norsteroids and oral contraceptives. Synthesis of (di)-norgestrel and ethinyl oestradiol. **14 Hrs**

3. Alkaloids

Definition nomenclature, occurrence, isolation, classification, general methods of structure elucidation. Synthesis and biosynthesis of the following alkaloids: Ephedrine, hygrine, coniine, cocaine cinchonine and morphine. Structure elucidation of papaverine, reserpine and ergotamine. Photochemical synthesis of Nuciferine, coradyline and tylophorine. **11 Hrs**

4. Porphyrins and vitamin B12

Detailed study of structure and synthesis of haemin, chlorophyll-a Vitamin-B_{12} (structure and synthesis from cobyric acid only). **8 Hrs**

5. Prostaglandins, Prostacyclins and thromboxanes

Introduction, nomenclature, classification and biological role of prostaglandins, prostacyclins and thromboxanes. 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, PGE_3 by Upjohn's approach. Synthesis of Prostacyclin I_2 and thromboxane A2. **8Hrs**

6. Insect pheromones

Introduction, classification. Pheromones in pest control. Synthesis of

a. Grandisol (component of boll weecil pheromone)
b. Farenal (trail pheromone of pharaoh's ants)
c. Brevicomin (pheromone from *Dendroitis brevicomis*)
d. (+) – Disparlure (gypsy moth sex pheromone)
e. 3, 11- Dimethyl-2 nonacosanone (pheromone of German cockroaches).
f. Bombykol (sex pheromone of silkworm moth).
g. Multistriatin (Elm bark beetle sex pheromone). **6Hrs**

SUGGESTED BOOKS

1. 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, Acadcmic 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. I to S. Natori & S.Nozoe, Academic Press, NY,1972.
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 poprphyrins and related compounds, L.R. Milgrom, Wiley Chichester,1995.
13. Interpetation of the UV spectra of natural products, A.I. Scott, Press, Oxford, 1964.
14. Spectral data of natural products Vol.I, K. Yamaguchi, Elsevier Publishing Co, London,1970
15. Chemistry of natural Products: Aunified approach, N.R.Krishnaswamy, University Press India, 1999.
16. Organic Chemistry, Volumes I and II, I L Finar, Longman,(1999)

MCH 334 Spectroscopy II **60 Hrs**

1. **Ultraviolet and visible spectroscopy**

   Instrumentation various electronic transitions(185-800 nm), Beer-Lambert's law, effect of solvent on electronic transitions, ultraviolet bands for carbonyl compounds, unsaturated carbonyl compounds, diens, conjugated polyenes. Woodward-Fieser rules for conjugated diens, carbonyl compounds and aromatics, steric effects, prediction of $\lambda_{max.}$. **10 Hrs**

2. **Infrared spectroscopy**

   Instrumentation. Characteristic vibrational frequencies of organic functional groups. Effect of hydrogen bonding and solvent effects on the vibrational frequencies, overtones, combination bands and Fermi resonance. Application of Raman spectroscopy as a complimentary technique to IR in structure analysis. Problems using UV and IR. **10 Hrs**

3. **NMR Spectroscopy**

   Introduction-Fourier transform technique, chemical shift, spin-spin interaction, shielding mechanism, chemical shift values and correlation for protons bonded to carbon. Chemical exchange, effect of deuteration- spin-spin interactions (first order spectra) stereochemistry, hindered rotation, Karplus curve. Simplification of complex spectra, nuclear magnetic double resonance, chemical shift reagents, solvent effects, nuclear overhauser effect (NOE) and DEPT. ^{13}CNMR spectral analysis. Problems involving PMR and CMR (separately and combined)

   Two dimensional NMR spectroscopy - COSY, NOESY, INADEQUATE. **18 Hrs**

4. Mass Spectrometry

Introduction, instrumentation, ion production – EI, CI, FD, MALDI and FAB, Factors affecting fragmentation, ion analysis, ion abundance. Mass spectral fragmentation of organic compounds, molecular ion peak, metastable peak, McLafferty rearrangement. Nitrogen rule. Use of HRMS to determine exact molecular formulae. Problems. **11 Hrs**

5. Composite Problems

Problems involving the application of the above spectroscopic techniques for structural elucidation of organic molecules. **11 Hrs**

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. Lapman 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, New York, 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, New York, 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. Instrumental methods of analysis, H.H. Willard, L.L. Merrit, J.A. Dean and F.A. Settle, CBS Publishers and Distributors, 1986.
16. Fundamentals of molecular spectroscopy, 4th edn., C.N. Banwell and E.M. McCash, Tata McGraw-Hill, New Delhi, 1999.

MCH 351 Organic Chemistry Practical – I

I Qualitative Analysis

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

II Quantitative analysis

1. Determination of equivalent weight of carboxylic acids.
2. Saponification value of oil.
3. Estimation of glucose.
4. Iodine value of oil.
5. Estimation of nitro group by reduction using $SnCl_2$.
6. Estimation of nitrogen by Kjeldahl's method.
7. Determination of molecular weight of dihydroxy phenol.

SUGGESTED BOOKS

1. Text book of practical organic chemistry – A. I. Vogel, 1996.
2. Text books of quantitative organic analysis – A.I. Vogel, 1996.
3. A handbook of organic analysis – Clarke and Hayes, 1964.
4. Comprehensive practical organic chemistry: Preparation and quantitative analysis, V.K. Ahluwalia, R. Aggarwal, Universities Press (India), 2000.
5. Comprehensive practical organic chemistry: Qualitative analysis, V.K. Ahluwalia, S. Dhingra, Universities Press (India), 2000.

6. An advanced course in practical chemistry, A. Ghoshal, B. Mahapatra and A. Kr. Nad, New central book agency, Calcutta, 2000.
7. Practical organic chemistry (Quantitative analysis), B.B. Dey, M.V. Sitaraman and T.R. Govindachari, Allied publishers, new Delhi, 1992.

MCH 352 Organic Chemistry Practical – II

I Preparation

Preparation of the following compounds:

1. *p* – Nitro aniline from acetanilide.
2. *p* – Bromoaniline from acetanilide.
3. *m* – Nitro benzoic acid from methyl benzoate.
4. Anthranilic acid from phthalic anhydride.
5. Cannizarro reaction: Benzaldehyde
6. Fries rearrangement: Phenyl acetate
7. Friedel - Crafts reaction
8. Claisen–Schmidt reaction

II Extractions and Separations (Preliminary chromatographic Techniques)

Extractions

1. Extraction of piperine from pepper.
2. Extraction of caffeine from tea leaves.
3. Extraction of (+)-limonene from citrus rinds.
4. Extraction of azelaic from caster oil.

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.

SUGGESTED BOOKS

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. A handbook of organic analysis – Clarke and Hayes, 1964.
5. Comprehensive practical organic chemistry: Preparation and quantitative analysis, V.K. Ahluwalia, R. Aggarwal, Universities Press (India), 2000.
6. Comprehensive practical organic chemistry: Qualitative analysis, V.K. Ahluwalia, S. Dhingra, Universities Press (India), 2000.
7. An advanced course in practical chemistry, A. Ghoshal, B. Mahapatra and A. Kr. Nad, New central book agency, Calcutta, 2000.
8. Advanced practical organic chemistry, J. Mohan, Vol . I and II, Himalaya Publishing House, 1992.
9. Practical organic chemistry (Quantitative analysis), B.B. Dey, M V Sitaraman and T R Govindachari, Allied Publishers, New Delhi, 1992.
10. Laboratory techniques in organic chemistry, V K Ahluwalia, Pooja Bhagat and Renu Aggarwal, I K international Publishing House, New Delhi, 2005.
11. Intermediates for organic synthesis, V K Ahluwalia, Pooja Bhagat, Ramesh Chandra and Renu Aggarwal, I K International Publishing House, New Delhi, 2005.

FOURTH SEMESTER

MCH 431 Organometallic Chemistry **60 Hrs**

1. **Organometallic Complexes**

   Stability and decomposition pathways, classification of ligands, Nomenclature of Organometallic complexes, 16-and 18-electron rules, Electron counting-covalent and ionic models. **6 Hrs**

2. **Organometallic Compounds of main group elements**

   Group trends-Synthesis, structure and bonding in Li, Be, Mg, and Al alkyls. **8 Hrs**

3. **Synthesis, Structure, Bonding and decomplexation reactions of organotransition metal complexes having σ- and π -M-C bonds**

   σ -Bonded systems involving carbonyls, carbenes and carbines. π-bonded systems involving dihapto to octohapto ligands like acetylene, olefins, allyl moieties, butadiene, cyclobutadiene, cyclopentadiene, arenes, cyclohexa and cycloheptadienyl moieties, cyclohepta and cyclooctatrienes, cyclooctatetraene moieties. Fluxional behavior of organometallic compounds, cyclometallation and ring slippage reactions, activation of small molecules (H_2 and CO). **14 Hrs**

4. **Isoelectronic and isolobal concepts**

   Structure and bonding in carbonyl clusters, Wade-Mingos-Lauher rules, cluster valence electron count. **5 Hrs**

5. Chemistry of organotransition metal complexes

General introduction: Use of organometallics as protecting and stabilizing groups. Organometallics as electrophiles and nucleophiles. Organometallics in coupling and cyclisation reactions. Organometallics in isomerisation, oxidation and reduction reactions. Use of zirconium, iron, cobalt, nickel and palladium complexes in the synthesis of carbonyl compounds. **16 Hrs**

6. Use of other organometallics in organic synthesis

Use of organozinc, organocadmium, organolithium, organocopper (Gilman regents), organoselenium, organoaluminium, organosilicon, organogermanium, organocerium and organomercurials in organic synthesis. **11 Hrs**

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.
6. Organometallics, Vol. 1 & 2, M. Bochmann, Oxford Chemistry Primers, 1994.
7. Advanced organic chemistry, J. March, 4th Edn. John Wiley, 1999.
8. Organotransition metal chemistry, S.G. Davies, Pergamon Press, Oxford, 1982.

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MCH 432 Stereochemistry and Retro synthetic Analysis 60 Hrs

I Stereochemistry

1. Optical activity in the absence of chiral atoms

Chirality in allenes, alkylidene cycloalkanes, spiranes, biphenyls, adamentanes, cyclophanes, *trans*-cyclooctene, catenanes, rotaxanes and helicenes, assignment of R, S – configuration to these classes of compounds. **7 Hrs**

2. Optical activity due to the presence of 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. **5Hrs**

3. Methods of Determining Absolute Configuration

a) Chemical correlation:
   i) without affecting bonds attached to a stereo center and
   ii) affecting bonds attached to a stereo center in a predictable manner.
b) Optical rotatory dispersion: α-axial haloketone rule and octant rule, application of these rules in the determination of absolute configuration of cyclohexanones, decalones and cholestanones.
c) Study of quasi-racemates.
d) Anomalous X-ray Scattering technique. **7 Hrs**

4. Transannular reactions

Conformational analysis and trasnannular reactions of medium rings: Hydrolysis of medium ring epoxides and bromination of $C_8 - C_{10}$ cyclic dienes. **3 Hrs**

II Retrosynthetic analysis

1. Disconnection Approach

Introduction to synthons and synthetic equivalents, disconnection approach. Basic principles and terminologies used in disconnection approach. One group C–X and two groups C–X disconnections. Chemoselectivity, reversal of polarity, cyclisation reactions. **8 Hrs**

2. Protecting groups

Principle of protection of alcohol, amine, acid and carbonyl groups. **5 Hrs**

3. C-C one group and C-C two group disconnections

Synthesis of alcohols, carbonyl compounds and alkenes. Use of acetylides and aliphatic nitro compounds inorganic synthesis. Diels–Alder reaction, 1,3-difunctionalised compounds, α,β-unsaturated compounds, carbonyl compounds condensations, 1,5-difunctionalised compounds. Michael addition and Robinson annelation. **12 Hrs**

4. Ring Synthesis

Synthesis of saturated heterocycles, and 3-, 4-, 5- and 6- membered rings. **5 Hrs**

5. Synthesis of some complex molecules

Application of the above in the synthesis of following compounds: Aromadendrene, Copaene, Longifolene, Juvabione, α - / β - Sinensals, benziodarone, fredericamycin and Lycorane. **8 Hrs**

SUGGESTED BOOKS

1. Streochemistry of carbon compounds, E.L. Eliel, S.H. Wilen & L.N. Mander, John Wiley & Sons, 1994.
2. Streochemistry, Potapov, MIR, Mescow, 1984.

3. Streochemistry, Nasipuri, D, New Age, 1999.
4. Advanced organic chemistry, J. March, 4th Edn. John Wiley, 1999.
5. Organic Chirality, 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 & 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 & M. Wills, Oxford University Press, 1995.
11. Organic synthesis: Concepts, Methods & starting materials, J. Furhfop & G. Penzilli, Verlag VCH.
12. Principals of organic synthesis, R. Norman & J.M. Coxon, Blackie Academic & Professional.
13. Advanced organic chemistry Part B, F.A. Carrey & J. Sundberg, Plenum Press, 1999.
14. Organic chemistry Vol. 2, 6th Edn., I.L. Finar, Longman, 1992.

MCH 433 Organic Synthesis II 60 Hrs

1. **Nonbenzenoid and polycyclic aromatic compounds**

   Nonbenzenoid aromatic compounds: Introduction, synthesis of cyclopropenyl cations, cyclobutadienyl dications, cyclopentadienyl anions, cycloheptatrienium cation, cyclooctatetraenyl dication, [10], [14], and [18]- annulenes, azulene and their reactions.

   Polycyclic aromatic compounds: Introduction, nomenclature, preparation of anthracene, phenanthrene, chrysene, picene, pyrene, perylene, coronene and circumanthracene. Reactions of anthracene and phenanthrene. **10 Hrs**

2. **Pesticides and insecticides**

   Introduction, classification. Naturally occurring insecticides: Rotenones, pyrethrins, precocenes. Synthetic insecticides: properties and synthesis of DDT, BHC, chlorodane, aldrin, dieldrin, parathion and malathion. Use of the following in the control of pests and insects: Fumigants, nematicides, acaricides, hormones (juvenile hormone), insect repellents, molluscicides and rodenticides. **6Hrs**

3. **Organic synthesis under the influence of ultrasound**

   Introduction, instrumentation, the phenomenon of cavitation. Homogeneous and heterogeneous (liquid-liquid and liquid-solid) reactions, Sonochemical esterification, substitution, addition, oxidation, reduction and coupling reactions. **5 Hrs**

4. **Microwaves in organic synthesis**

Introduction, reaction vessel, reaction medium, concept, specific effects, atom efficiency, % atom utilization, advantages and limitations. N-alkylation and alkylation of active methylene compounds, condensation of active methylene compounds with aldehydes. Synthesis of Ibuprofen by BHC and BOOTS approaches. Diels-Alder reaction, Leuckardt reductive amination of ketones, oxidation of alcohols and sulfides. Ionic-liquids: structure and applications. **5 Hrs**

5. Phase transfer catalysis and Crown ethers

Phase transfer catalysis: Introduction, definition, mechanism of phase transfer catalysis, advantages and types of phase transfer catalysts. Preparation of catalysts and applications: substitution, elimination, addition, condensation, oxidation and reduction reactions.

Crown ethers: Introduction, nomenclature, features, nature of donor site. General synthesis of Crown ethers. Synthetic applications- alkylation, anhydride formation, generation of carbenes, aromatic substitution and displacement reactions. Cation deactivation reactions. **10 Hrs**

6. Polymer supported reagents and synthesis

Introduction- properties of polymer support, advantages of polymer supported reagents and choice of polymers. Application: Substrate covalently bound to the support- synthesis of oligosaccharides, intramolecular cyclisation reactions, solid state Edman degradation. Reagent linked to a polymeric material-diazotransfer reaction, Wittig reaction, oxidation with polymer bound per acid. Polymer supported catalytic reactions–acetal from polymer supported $AlCl_3$, polymer bound phase transfer reagents in organic synthesis. **10 Hrs**

7. Asymmetric Synthesis

Defintion, importance, energy considerations, advantages and limitations. Methods of determination of enantiomeric excess.

Synthesis and applications of oxazaborolidines, IPC-BBN, IPC_2BH, (S)-BINAP-DIAMINE and (R)-BINAL-H.

Use of (R,R)-DIPAMP, (S,S)-CHIRAPHOS, (R,R)-DIOP, SAMP RAMP, S-Proline, S-PBMgCl, (−)-$BOACl_2$, (+) and (−)-DET and MRN as catalysts in asymmetric synthesis. **14 Hrs**

SUGGESTED BOOKS

1. Polymer science, V.R Gowariker, N.V. Vishwanathan & J. Sreedhar, Wiley Eastern Ltd. 1986
2. Polymer: chemistry & physics of modern materials J.M.G.Cowie, International Text Books Co Ltd 1973
3. Chemical process industrial chemistry , 3rd Edn. Mc Graw- Hill,1967.
4. Riegels handbook of industrial chemistry, James A. Kent , 7th edn.1974
5. Basic organic chemistry part-v: industrial products , J.M Tedder , A Nechuvatal & A.H. Jubb, John wiley & sons 1975
6. A textbook of organic chemistry, V K Ahluwalia and M. Goyal, Narosa publishing House , New Delhi, 2000
7. Organic synthesis: special techniques, V K Ahluwalia and R Aggarwal, Narosa, New Delhi, 2001
8. Green chemistry, environment friendly alternatives, R. Sanghi and M M Srivastava, Narosa, New Delhi 2003
9. Green Chemistry- an introduction text, Royal Society of chemistry , UK, 2002
10. Stereochemistry of carbon compounds, E.L .Eliel, S.H.Wilen and L.N Mander, John Wiley & sons, 1994
11. Stereochemistry, Potapov, MIR Moscow,1984.
12. Stereochemistry,Nasipuri, D ,New Age,1999
13. Advanced organic chemistry,J.march,4th Edn John Wiley 1999
14. The text book of polymer science, F.W Billmeyer, Jr, Wiley intersciences,1984.
15. Principles and applications of asymmetric synthesis, G D Lin, Y M LI ,and A S C Chan, Wiley intersciences, 2001.

MCH 434 Medicinal Organic Chemistry 60 Hrs

Introduction

Chemotherapy, pharmacokinetics, pharmacodynamics, metabolites and antimetabolites. Prodrugs and soft drugs, agonists and antagonists. Concept of drug receptor. Elementary treatment of drug receptor interaction. Quantitative structure activity relationship (QSAR). Theories of drug activity: Occupancy theory, rate theory and induced fit theory. Computer-aided drug design and molecular modeling. General Principles of dosage form design and drug administration. **8 Hrs**

Mechanism of drug action and the synthesis of the following classes of drugs (interconversions as applicable):

1. **Antipyretics, analgesics and Antiinflammatory Drugs**

   Aspirin, paracetamol, Phenacetin, novalgin, phenylbutazone, ibuprofen, naproxen.

   3 Hrs

2. **Antibiotics**

   Pencillin-G, ampicillin, amoxicillin, chloramphenicol, cephalosporins, tetracyclins-aureomycin and terramycin, streptomycin. **8 Hrs**

3. **Antidiabetics**

Insulin and oral hypoglycemic agents: Structure of insulin, glibenclamide, metformin and ciglitazone. **3 Hrs**

4. Antihistamines

Methapyrilene, chlorpheniramine **3 Hrs**

5. Antineoplastic agents

Mechlorethamine, cyclophosphamide, melphalan, uracil mustards and 6-mercaptopurine. **5 Hrs**

6. Antivirals

Acyclovir, Amanditidine, Rimantidine and Zidovudine. **3 Hrs**

7. Cardiovascular drugs

Amyl nitrite, sobitite, guanidine, verapamil, methyldopa. **5 Hrs**

8. Local antiinfective drugs

Suphonamides, furazolidone, nalidixic acid, ciprofloxacin, norfloxacin, dapsone, aminosalicylic acid, isoniacid, ethionamide, ethambutal, griseofulvin, chloroquin and primaquin. **10 Hrs**

10. Psychoactive drugs- the chemotherapy of the mind

Phenobarbital, pethidine, methadone, chlodiazepoxide, diazepam, meprobamate, chloropromacine, alprazolam, phenytoin, ethosuximide, trimethadione, barbiturates, thiopental sodium, glutethimide and caffeine. Brief account of β-LPH and its relation to : β-endorphin, MSH and ACTH.

Brief discussion on the recent developments chemotherapy. Lead compounds and their isolation from natural and synthetic sources. Generics and analogous. Green chemistry in the manufacture of drugs. **12 Hrs**

SUGGESTED BOOKS

1. Introduction to medicinal chemistry, A. Gringuage, Wiley-VCH
2. Wilson and Gisvold's Text book of organic medicinal and pharmaceutical chemistry, Ed Robert F. Dorge.
3. An introductuion to drug design., S.S. Pandey and J.R. Dimmock, New Age International.
4. Burger's medicinal chemistry and drug discovery, vol-1(chapter 9 and 14) Ed.M.E. Wolff, John Wiely.
5. Godd man and Gilman's pharmacological basis of therapeutics,McGraw-Hill.
6. The organic chemistry of drug design and drug action, R.B.Silverman, Academic Press.
7. Strategies for organic drug synthesis and design, D. Lednicer, John Wiley.
8. Medicinal Chemistry, A Kar, Wiely, 2000.
9. Synthetic drugs, G.R. Chatwal, Himalaya, New Delhi, 1995.
10. Comprehensive organic chemistry, vol.5 (Antibiotics). D.H.R. Barton, W.D.Ollis, Pergamon press, Ny, 1979.
11. Instant notes on medicinal chemistry, P.Graham, Viva, New Delhi,2002.

CHE 451 Organic Chemistry Practical –III

I Preparations

1. Anthrone from Anthracene.
2. Benzilic acid from benzaldehyde
3. Preparation of NBS from succinic acid and its application in allylic bromination reactions.
4. Preparation of benzpinacolone from benzophenone.
5. Preparation of 2-phenylindole from phenylhydrazine.
6. Preparation of 2,4,5-triphenyloxazole from bezoin.
7. Sand Meyer reaction: *p*–Chlorotoluene from *p*–toluidine
8. Preparation of S–benzylisothiuronium chloride.

II Instrumental Methods in Organic Analysis

1. Recording of spectra using UV, IR, NMR and GC_MS techniques for the compounds prepared in MCH-351(Organic Practical-I), MCH-352 (Organic Practical-II), MCH-451 (Organic Practical-III).
2. Structural elucidation of organic compounds with spectra provided by instructors/examiners.

SUGGESTED BOOKS

1. Text book of practical organic chemistry – A. I. Vogel, 1996.

2. A handbook of organic analysis – Clarke and Hayes, 1964.
3. Comprehensive practical organic chemistry: Preparation and quantitative analysis, V.K. Ahluwalia, R. Aggarwal, Universities Press (India), 2000.
4. Comprehensive practical organic chemistry: Qualitative analysis, V.K. Ahluwalia, S. Dhingra, Universities Press (India), 2000.
5. An advanced course in practical chemistry, A. Ghoshal, B. Mahapatra and A. Kr. Nad, New central book agency, Calcutta, 2000.
6. Advanced practical organic chemistry, J. Mohan, Vol . I and II, Himalaya Publishing House, 1992.

MCH 452 Industrial project work