MANONMANIAM SUNDARANAR UNIVERSITY

DEPARTMENT OF CHEMISTRY

STRUCTURE OF M.Sc. CHEMISTRY PROGRAM

For the academic year 2018-2019

Preamble

The emerging Chemical Technologies are highly science based. A Chemist cannot isolate himself from other disciplines. The practice of Chemistry over a span of more than a century has created unavoidable impacts of human environment. The adverse effects were particularly noted during last few decades. The concept of sustainable development is now well accepted. The principles and applications of Chemistry should be learnt on this background.

Necessity

The purpose of post-graduate education in Science is to create highly skilled manpower in specific areas, which will lead to generation of new knowledge and creation of wealth for the country. Chemistry is a fundamental science and has contributed immensely to the improvement of the life of human beings by providing many of human requirements and essentialities.

Importance

Chemistry is important to the world economy as well. The developments in Chemistry during last few decades are phenomenal. It is also seen that these developments are crossing the traditional vertical boundaries of scientific disciplines; the more inclination is seen towards biological sciences. New branches of Chemistry are emerging and gaining importance, Such as bioorganic chemistry, Materials chemistry, computational chemistry etc. The practice of Chemistry at industrial scale also is undergoing radical changes and is more or more based on deep understanding the chemical phenomena.

Objectives

i. To impart training in Chemistry at advanced level in a more holistic way and enthuse the students for the subject.
ii. To train the students to make them confident and capable of accepting any challenge in Chemistry.
iii. To give a flavour of research in Chemistry and train the students for research career.
iv. To abreast the students about the current status and new developments in Chemistry.
v. To make the students aware of the impact of Chemistry on environment and imbibe the concept of sustainable developments.
vi. To educate the students with respect to skills and knowledge to practice chemistry in way that are benign to health and environment.

Outcome

After completing the M.Sc. program the students will be able to

i. Pursue research program
ii. Qualify as Chemist/Scientist in various industries and research institutions

Eligibility Norms

B.Sc. degree in Chemistry or any other equivalent Bachelor Degree is eligible for the admission in M.Sc. Chemistry program.

Admission Procedure:

Admission will be based on (i) the total marks obtained in the entrance test (50%) and the qualifying B.Sc. degree examination (50%) (merit list for a Total of 100 marks) and (ii) by following the govt. norms of reservation.

Scheme of Examination and question pattern

Time: 3 hours Max. marks:75

Part A	:	10 questions full of Objective type WITHOUT multiple choice. Two questions from each unit of a paper. Each question carries one mark	10 x 1=10 marks
Part B	:	5 descriptive questions, of either a or b type (internal choice). One question is from each unit. Each question carries 5 marks	5 x 5 = 25 marks
Part C	:	5 descriptive questions of either a or b type (internal choice). One question is from each unit. Each question carries 8 marks.	5 x 8 = 40 marks

Course Weight:

In each of the courses, credits will be assigned on the basis of the lectures, tutorials / lab work and other forms of learning in a 15 week schedule.

1. One credit for each lecture hr. per week
2. One credit for each tutorial hr. per week
3. One credit for every two hrs. of Lab or Practical Work per week

Internal /External Distribution of Marks

For all theory papers, the Internal / External distribution of Mark will be 25: 75 (Total = 100).

The 25 marks for the internal component has been divided as follows:

3 compulsory tests, out of which average of the best two tests	= 15 marks
Seminar	= 5 marks
Assignment	= 5 marks
	_____

Total =25 marks

For theory **Paper No. 16,** i.e. Literature Survey and Research Methodology (Seminar paper related to project work) there will be Internal only; no University final examination. Being a Paper related to their project work, the students will be evaluated by continuous internal assessment only, consisting of 3 examinations, 3 seminars and mark distribution will be

3 compulsory examinations, out of which average of the best two examination	=	75 marks
3 compulsory seminars, out of which average of the best two Seminars	=	25 marks
Total	=	100 marks

The 3 seminars will be conducted jointly by the guide and another faculty member of Chemistry.

For all Practical papers the examination time shall be 6 hours and the Internal / External distribution of Marks will be 25: 75 (Total = 100) respectively.

PROJECT

Project for IV semester shall be an INDIVIDUAL project. Project evaluation will be done by Guide and another faculty member of the department. Viva voce Examination for the project students will be conducted jointly by the same examiners who evaluated the project report.

$$\text{Cumulative weighted average of marks} = \frac{\sum(\text{Marks x Credits})}{\sum \text{Credits}}$$

$$\text{Cumulative weighted average Grade Points} = \frac{\sum(\text{Grade Point x Credits})}{\sum \text{Credits}}$$

Course Structure of M.Sc Chemistry Program

The course shall consist of 90 credits distributed in four semesters as under:

Sl. No.	Course code	Papers	Credits	Hours
I Semester				
1	MCHC11	Organic Chemistry I	4	4
2	MCHC12	Inorganic Chemistry I	4	4
3	MCHC13	Physical Chemistry I	4	4
4	MCHC14	Computer Applications in Chemistry	4	4
5	MCHL11	Organic Chemistry Practical - I	2	4
6	MCHL12	Inorganic Chemistry Practical - I	2	4
		Total	**20**	**24**
II Semester				
7	MCHC21	Organic Chemistry II	4	4
8	MCHC22	Inorganic Chemistry II	4	4
9	MCHC23	Physical Chemistry II	4	4
10	----	Supportive course paper I –to be offered by other depts.	3	3
11	MCHL21	Organic Chemistry Practical –II	2	4
12	MCHL22	Inorganic Chemistry Practical- II	2	4
		Total	**19**	**23**
III Semester				
13	MCHC31	Organic Chemistry III	4	4
14	MCHC32	Inorganic Chemistry III	4	4
15	MCHC33	Physical Chemistry III	4	4
16	MCHP31	Literature Survey and Research Methodology (Seminar paper related to project work)	4	4
17	MOOCS	Supportive Paper II - to be offered by moocs	3	3
18	MCHL31	Physical Chemistry Practical – I	2	4
19	MCHL32	Physical Chemistry Practical – II	2	4
		Total	**23**	**27**

IV Semester				
20	MCHOEA/B/C	Organic - Elective Paper –(One paper out of 3 offered)	3	3
21	MCHIEA/ B/C	Inorganic - Elective Paper - (One paper out of 3 offered)	3	3
22	MCHPEA/B/C	Physical - Elective Paper – (One paper out of 3 offered)	3	3
23	MCHL41	Organic Practical III – Advanced Organic Chemical Analysis	2	4
24	MCHL42	Inorganic Practical III – Advanced Inorganic Chemical Analysis	2	4
25	MCHL43	Physical Practical III – Advanced Physical method of Chemical Analysis	2	4
26	MCHP41	Project	13	13
		Total	**28**	**34**
		Grand Total	**90**	**108**

SEMESTER I

ORGANIC CHEMISTRY – I

MCHC11		
L (hrs)	Credits	Course
60	4	Core

Unit I Chemical bonding and structure: **(12 hrs.)**

a) Inductive effect - mesomeric effect - steric inhibition of resonance - 'pπ-dπ' bonding - hyperconjugation -cross-conjugation - hydrogen bonding -acidity, basicity, factors affecting the strength of acids and bases- hard and soft acids and bases.

b) Reactive Intermediates: Formation, structure, and stabilization of carbocations, carbanions, free radicals, carbenes, and nitrenes.

Unit II Introduction to reaction mechanism: **(12 hrs.)**

Kinetic and thermodynamic requirements, kinetic and thermodynamic control, Hammond Postulate, microscopic reversibility, Curtin-Hammet principle, energy profile diagram, intermediates *Vs* transition states.

Methods of determining reaction mechanism: Nonkinetic methods-Identification of products, intermediates, stereochemistry, crossover experiments, nonkinetic isotopic labeling. Kinetic methods-order, molecularity, influence of ionic strength (salt effects), primary and secondary isotopic effects.

Unit III Aromaticity: **(10 hrs.)**

Huckel's Rule-Craig's Rule-concept of aromaticity, homoaromaticity and antiaromaticity - systems of 2, 4, 8 and 10-π electrons. large cyclic π systems-aromaticity of azulenes, annulenes, sydnones and tropolones.

Unit IV Stereoisomerism: **(16 hrs.)**

Optical isomerism: Symmetry elements and chirality, necessary and sufficient condition for chirality - concept of prochirality - enantiotropic and diasterotropic-Fischer, Sawhorse and Newmann projection formulae and their interconversions-calculations of number of stereoisomers - R, S-notations- atropisomerism - molecular dissymmetry - optical activity of allenes and spiranes.

Geometrical isomerism: E-Z nomenclature - stereoisomerism in monocyclic compounds upto six-membered rings. Conformation and reactivity of six-membered ring systems.

Unit V Proteins and lipids: **(10 hrs.)**

General methods of synthesis and reactions of amino acids peptides-solid phase polypeptide synthesis (Merrifield method)

Chemical and enzymatic hydrolysis of proteins to peptides, amino acid sequencing. Secondary structure of proteins, forces responsible for holding of secondary structures, α- helix, β-sheets, super secondary structure. Tertiary structure and Quaternary structure.

Lipids:

Lipids-classification,Fat and oils, chemical properties - formation of micelle, fatty acids, glycolipids, phospholipids.

References

1. F. A. Carey and R. A. Sundberg, Advanced Organic Chemistry, Part A: Structure and Mechanisms, 5th Edition, Springer, New York, 2007.
2. Stereochemistry of Carbon Compounds by E. J. Eliel, McGraw Hill
3. Organic Chemistry by S. H. Pine, McGraw Hill,1987
4. Stereochemistry of Organic Compounds by D. Nasipuri, Wiley,1994.
5. Robert E. Gawley, Jeffrey Aube, Principles of Asymmetric Synthesis, pergamon, 2nd edition, 1996
6. V.K. Ahluwalia and R.K. Parashar, Organic Reaction Mechanisms, Narosa Publishing House, 2002.
7. Stereochemistry, D. G. Morris, , RSC Tutorial Chemistry Text 1, 2001.
8. E. L. Eliel and S. H. Wilen, Stereochemistry of Organic Compounds, John Wiley & Sons, New York, 1994.
9. D. G. Morris, Stereochemistry, RSC Tutorial Chemistry Text 1, 2001
10. J. Kirby, Stereoelectronic effects, Oxford Chemistry Primers, 2011.
11. Steric and Stereoelectronic Effects in Organic Chemistry, V. K. Yadav, Springer, 2016.

MCHC12		
L (hrs)	Credits	Course
60	4	Core

INORGANIC CHEMISTRY – I

Unit I Chemical Bonding and Stereochemistry (12 hrs.)

Nature of covalent bond : MO theory of polyatomic molecules, ionic bond and its energetics : lattice energy – Born Lande equation and Born Haber cycle – covalent character in ionic bond - partial ionic character from dipole moment and electronegativity data.

VSEPR theory – the concept of multicentre bond and structure as applied to boron hydrides. Noble gas chemistry, their halides and pseudohalides – structure and bonding.

Unit II Redox potential and Inorganic polymers (12 hrs.)

Applications of redox potential to inorganic reactions - factors affecting redox potential.Catenation and heterocatenation – Three dimensional silicates, one dimensional conductors, isopoly and heteropolyacids, borazines, phosphazenes, S –N ring compounds, phosphorous cage compounds, binuclear metal clusters : synthesis, structure and bonding of $[Re_2Cl_8]^{2-}$. Oxyacids of Selenium and Tellurium.

Unit III Coordination Chemistry – I (14 hrs.)

VB, CF and MO theories of complexes with four and six coordination numbers – CFSE – factors affecting the magnitude of 10 Dq values - spectrochemical series - applications of CFT - site preferences in spinels - nephelauxetic effect - π bonding and MO theory - static and dynamic Jahn-Tellar behaviour.

Different types of magnetic behaviour, magnetic moment determination by Guoy and Faraday methods, spin only value - quenching of orbital angular momentum - spin-orbit coupling - determination of geometry of Co and Ni complexes from magnetic data - spin crossover phenomenon - magnetic properties of lanthanides.

Unit IV Electronic Spectroscopy (12 hrs.)

L-S coupling scheme, microstates, term symbols and Hund's rule - splitting of terms, hole formalism and selection rules - Orgel and Tanabe – Sugano diagrams - evaluation of 10 Dq and β for octahedral d^2, d^6 and d^8 systems - effect of distortion and spin-orbit coupling on the spectra - charge-transfer spectra - electronic spectra of lanthanide complexes.

Optical isomerism in octahedral complexes - absolute configuration of chelate complexes from ORD and CD techniques.

Unit V Nuclear Chemistry (10 hrs.)

Radioactive decay and equilibrium, nuclear structure and models; types of nuclear reactions – Q value, cross section – fission and fusion; fission products and fission yields, nuclear reactors, nuclear power projects in India - radioactive techniques (radiometric titrations, isotope dilution method and neutron activation analysis), counting techniques (G.M., ionization, scintillation and proportional counters)

References:

1. J.E. Huheey, E.A. Keiter and R.L. Keier, Inorganic Chemistry, Harper and Row, 4th Edn., 1993.
2. F.A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, John Wiley & Sons, 5th Edn., 1988.
3. B.E. Douglas, D.H. McDaniel and J.J. Alexander, Concepts and Models of Inorganic Chemistry, John Wiley & Sons, 2 Edn. 1983.
4. R.S. Drago, Physical Methods in Chemistry, W.B. Saunders, 1997.
5. E.A. V. Ebsworth et al., Structural Methods in Inorganic Chemistry, ELBS 1987.
6. J.D. Lee, Concise Inorganic Chemistry, ELBS 1990.
7. M.C. Day, Jr., and J. Selbin, Theoretical Inorganic Chemistry, East West Press.
8. S. Glasstone, Source book on atomic energy, East West press, 3rd Edn. 1967.
9. H.J. Arniker, Essentials of Nuclear Chemistry, Wiley Eastern, 1983.
10. M.G. Friedlander, J.M. Kennedy, E.S. Macian and J.M. Miller, Nuclear and Radiochemistry, 3rd Edn. John Wiley & Sons, 1981.
11. M.G. Arora and M. Singh, Nuclear Chemistry, Anmol Publications, 1994.

PHYSICAL CHEMISTRY-I

Chemical Kinetics, Thermodynamics and Electrochemistry

MCHC13		
L (hrs)	Credits	Course
60	4	Core

Unit I Chemical Kinetics –I **(12 hrs.)**

Absolute reaction rate theory (ARRT) including thermodynamic treatment – application of ARRT to simple bimolecular processes – potential energy surfaces – kinetic isotope effect- termolecular reactions; theory of unimolecular reactions – Lindemann's theory , Hindshelwood theory, KRR theory, KRRM theory and Slater's theory.

Chain reactions –general characteristics – kinetic – thermal reaction between H_2 and Br_2, thermal decomposition of N_2O_5, formation and decomposition of phosgene-Rice-Herzfeld mechanisms – application to reactions of 0.5, 1 and 1.5 order; explosions – hydrogen-oxygen reaction.

Unit II Chemical Kinetics- II (**12 hrs.)**

Kinetics of reactions in solution –ion-ion and ion-dipole reaction – role of dielectric constant, effect of ionic strength and influence of pressure on the reaction rates.

Homogeneous catalysis – acid-base catalysis – methods for investigating acid-base catalysis – salt effect in acid base catalysis – mechanisms of acid-base catalysis; acidity functions and their importance; Bronsted catalysis law.

Enzyme kinetics – effect of substrate concentration – Michaelis-Menten law – Lineweaver –Burk and Eadie methods – effect of pH and temperature; inhibition competitive, uncompetitive and non-competitive inhibitions.

Unit III Thermodynamics I (**12 hrs.)**

Thermodynamics of systems of variable composition – partial molar properties-chemical potential –Gibbs Duhem equation – apparent molar properties-methods of determination of partial molar quantities, partial molar thermal properties – differential and integral heats of solution thermodynamics of mixing

Thermodynamic properties of real gases – fugacity concept – determination of fugacity – real amd mixture of gases – Lewis – Randall rule. Nernst heat theorem – different forms of stating the third law – thermodynamic quantities at absolute zero.

Unit IV Electrochemistry-I (**12 hrs.)**

Debye-Huckel-Onsager equation – derivation and experimental verification – Debye-Falkenhagen and Wien effect; activity and activity coefficient – Debye-Huckel

limiting law – derivation and verification – activity at appreciable concentration and extension of Debye-Huckel theory. Nernst equation – reduction system – electrochemical cells.

Electrodics – types of electrode – EMF and its measurements – application of EMF measurements – determination of thermodynamics parameters, equilibrium constant, solubility product and dissociation constant.

Unit V Electrochemistry – II **(12 hrs.)**

Kinetics of electrode processes – Butler Volmer equation – Tafel equation- electrical double layer – zetapotential – electrokinetic phenomena- over voltage – hydrogen over voltage – theories of over voltage; polarography – principle and applications; primary and secondary coulometric titration.

Passivity – electrochemical, chemical and mechanical passivity; corrosion – theories, methods of preventing corrosion; electrochemical processes as sources of energy – dry cells – storage batteries – fuel cells.

References:

1. K. J. Laidler, Chemical Kinetics, 2nd Edition, Tata McGraw-Hill, New Delhi, 1991.
2. K. J. Laidler, Theories of Chemical Reaction Rates, McGraw-Hill, New York, 1969.
3. D. V. Roberts, Enzyme Kinetics, Cambridge University Press, Cambridge, 1977.
4. J. C. Kuriacose, Catalysis, Macmillan India, Ltd., New Delhi, 1991.
5. W. J. Moore, Basic Physical Chemistry, Prentice Hall, 1986.
6. S. Glasstone, An introduction to Electrochemistry, Van Nostrand, New York, 1965.
7. J. D. M. Bockris, A.K.N. Reddy, Modern Electrochemistry, Vol. I & II, Plenum Press, New York, 3rd Reprint, 1977.
8. A. J. Bard, L.R. Faulkner, Electrochemical Methods: Fundamentals and Applications, John Wiley and Sons, New York, 1980.
9. R. Crow, Principles and Applications of Electrochemistry, Chapman and Hall, London, 1979.

COMPUTER APPLICATION

Computer Applications in Chemistry

MCHC14		
L (hrs)	Credits	Course
60	4	Core

Unit I **(12 hrs.)**

Introduction – Significant developments in the history of computers – computer generations – Components of a computer –block diagram-CPU, ALU, control units, memory unit, Memory –classification of memory devices, Main memory –semiconductor memory devices (RAM, ROM) – Secondary memory devices – magnetic disks (hard and floppy) – Peripheral devices – Input devices – keyboard keys and their uses-mouse; Output devices – VDU-printer and its classification; Hardware and software.

Classification of computers –based on working principle (analog and digital)-based on processing capabilities (micro, mini, mainframe and supercomputers); Computer software –system software and application software – computer languages (machine, assembly and high level)-assembly program, compiler and interpreter.

Unit II **(12 hrs.)**

Microsoft office 2007 – Word-Editing text-document formatting-reusable formatting with styles and templates- Tables and columns-Advanced page layout in word – automating information with fields – mail merge, labels and envelope.

Spreadsheet – excel – formatting worksheets and restricting data – calculating with formulae and functions – viewing and manipulating data with pivot tables.

Powerpoint – creating and editing slides – adding graphics, multimedia and special effects to slides – showing powerpoint presentations.

Unit III **(12 hrs.)**

C Programming – introduction – Character set in C – Style of C language-planning a C program – top down programming – C keywords – variables in C, local variables, global variables and formal parameters, constant in C- operations in C, input and output functions in C, loops in C language, arrays and points in C, continue statement and GO TO statement, break statement- storage classes in C – writing C program using various features of C language.

Unit IV **(12 hrs.)**

Programming – to compute the i) slope, intercept and correlation coefficient for the given set of data of straight line, ii) wavelength, frequency or energy for a wave, iii) lattice energy on the basis of Born Lande's equation, iv) number average and weight average molecular weight of a polymer, v) the value of maximum populous rotational

level, vi) rotational energy and rotational constant, vii) reduced mass and moment of inertia, viii) activation energy on the basis of Arrhenius equation, ix) rate constant for first, second and zero order kinetics, x) computation of value of absorbance on the basis of Lambert Beer's Law, xi) electronegativity of an atom from bond energy data using Pauling's relation, xii) calculation of λ_{max} for conjugated dienes and enones, xiii) to determine the molecular weight of organic compounds, xiv) to calculate the isoelectric points of amino acids xv) to compute statistical calculations of entropy.

Unit V **(12 hrs.)**

Cheminformatics – Introduction- definition, scope and use of cheminformatics, chemical database and chemical resources, search methods in cheminformatics; applications in drug discovery-evolution and process, major goals and strategies of drug discovery – development of the drug: the five classic steps, the current roles and uses of the computer in drug design – software using in drug design – preparing chemical mode through chemsketch and chemdraw softwares.

References

1. K. V. Raman, Computers in Chemistry, Tata McGraw Hill
2. K. Arora, Computer Applications in Chemistry, Anmol Publications Pvt. Ltd. 2004.
3. R. Kumari, Computers and their Applications to Chemistry, Narosa Publishing House Pvt. Ltd, Second Edition 2005.

PRACTICALS

ORGANIC CHEMISTRY PRACTICAL - I

MCHL11		
L (hrs)	Credits	Course
60	2	practical

1. Single stage preparations:

   Diels – Alder Reactiom, Bis – 2 – Naphthol, 1,2,3,4 – Tetrahydrocarbazole, Benzpinacol, Benzpinacolone, Aspirin, Phenol – formaldehyde resin, p – Nitroacetanilide, β – D – Glucopyranose, Fluorescein, p - Bromoacetanilide

2. Two stage preparation:

   Synthesis of Phthalamide, p – nitroaniine, p – Bromo aniline, M – nitrobenzoic acid

References

1. A. I. Vogel, A Text Book of Practical Organic Chemistry.
2. A. Ault, Techniques and Experiments for Organic Chemistry.
3. N. K. Vishnoi, Advanced Practical Organic Chemistry.
4. B. B. Dey and M.V. Sitaraman, Laboratory Manual of Organic Chemistry.
5. Raj K. Bansal, Laboratory Manual in Organic Chemistry.

INORGANIC CHEMISTRY PRACTICAL- I

MCHL12		
L (hrs)	Credits	Course
60	2	practical

1. Semi micro qualitative analysis of inorganic mixture containing two less-familiar cations.
   W, Tl, Se, Te, Mo, Ce, Th, Zr, Ti, V, U and Li
2. Complexometric titrations – Estimation of Cu, Zn and Mg by EDTA titration in the presence of either Pb or Ba; estimation after elimination of Pb or Ba.
3. Determination of Total hardness, Ca and Mg content of water by EDTA titration

References:

1. V.V. Ramanujam, 'Inorganic Semimicro Qualitative analysis, 3rd revised Edn, The National publishing Co., Chennai, 1988.
2. 'Vogel's Text Book of Quantitative Chemical Analysis', Eds. G.H. Jeffrey, J.Banett, J. Mendham and R.C. Denney, ELBS, 5th Edn. Reprint 1991.

SEMESTER II

MCHC21		
L (hrs)	Credits	Course
60	4	Core

ORGANIC CHEMISTRY - II

Unit I Nucleophilic substitution

(15 hrs.)

a) Aliphatic nucleophilic substitution

S_N1, S_N2, S_Ni, S_Ni' and tetrahedral mechanisms - ambident nucleophiles and ambident substrates - effect of substrate, attacking nucleophile, leaving group, and reaction medium - neighbouring group participation (NGP) - hydrolysis of esters.

b) Aromatic nucleophilic substitution:

S_NAr, S_N1 and benzyne mechanisms

Unit II Electrophilic substitution **(12 hrs.)**

a) Aliphatic electrophilic substitution:

S_E1, S_E2 and S_Ei mechanisms

b) Aromatic electrophilic substitution reactions:

Arenium ion and S_E1 mechanisms. Orientation and reactivity of monosubstituted benzene rings - ortho/para ratio - Ipso attack. Quantitative treatment - reactivity in the substrate - reactivity of the electrophile, effect of leaving group.

Unit III Asymmetric Synthesis **(15 hrs.)**

Chiral auxiliatries, methods of asymmetric induction – substrate, reagent and catalyst controlled reactions; determination of enantiometric and diastereomeric excess; enantio-discrimination. Resolution – optical and kinetic. Cram's rule, Prelog's rule-stereoselective and stereospecific syntheses.

Asymmetric reactions with mechanism: Aldol and related reactions including Cram's rule, Sharpless enantioselective epoxidation, hydroxylation, aminohydroxylation, Diels-Alder reactions.

Unit IV Elimination and Addition reactions **(10 hrs.)**

Elimination Reactions

E1, E2, E1CB mechanisms - stereochemistry of eliminations - elimination versus substitution - orientation of double bond - Sayzteff and Hoffman rules - pyrolytic eliminations - mechanism of pyrolysis of esters of carboxylic acids.

Addition reactions

Electrophilic, nucleophilic and free radical additions - Orientation and stereochemistry of addition of halogens and hydrogen halides to carbon-carbon

multiple bonds - hydroboration, Sharpless asymmetric epoxidation and hydroxylation - Addition to α, β - unsaturated carbonyl compounds.

Unit V Carbohydrates and Nucleic acids: (**08 hrs.)**

a) Carbohydrates: classification of carbohydrates, sugar and non-sugar compounds, ring structure of carbohydrates, amylose, cellulose, acetylation of carbohydrates, epimerisation, carbohydrates reaction with phosphoric acids and amines, Optical activity –mutarotation of glucose.

b) Nucleic acids: Structure and function of physiologically important nucleotides (c-AMP, ADP, ATP) and nucleic acids (DNA and RNA), replication, genetic code, protein biosynthesis, mutation.

References

1. F. A. Carey and R. A. Sundberg, Advanced Organic Chemistry, Part A: Structure and Mechanisms, 5th Edition, Springer, New York, 2007.
2. Stereochemistry of Carbon Compounds by E. J. Eliel, McGraw Hill
3. Organic Chemistry by S. H. Pine, McGraw Hill,1987
4. Stereochemistry of Organic Compounds by D. Nasipuri, Wiley,1994.
5. Robert E. Gawley, Jeffrey Aube, Principles of Asymmetric Synthesis, pergamon, 2nd edition, 1996
6. V.K. Ahluwalia and R.K. Parashar, Organic Reaction Mechanisms, Narosa Publishing House, 2002.
7. Stereochemistry, D. G. Morris, , RSC Tutorial Chemistry Text 1, 2001.
8. E. L. Eliel and S. H. Wilen, Stereochemistry of Organic Compounds, John Wiley & Sons, New York, 1994.
9. D. G. Morris, Stereochemistry, RSC Tutorial Chemistry Text 1, 2001
10. J. Kirby, Stereoelectronic effects, Oxford Chemistry Primers, 2011.
11. Steric and Stereoelectronic Effects in Organic Chemistry, V. K. Yadav, Springer, 2016.

INORGANIC CHEMISTRY – II

MCHC22		
L (hrs)	Credits	Course
60	4	Core

Unit I Coordination Chemistry II **(10 hrs.)**

Thermodynamic stability – stepwise and overall stability constants and their relationship – determination of stability constant by potentiometric and spectrophotometric methods, factors affecting stability : chelate effect, kinetic and thermodynamic template effects and their application in the synthesis of macrocyclic ligands; HSAB concept : applications and theoretical basis, characterization of stabilities of mixed ligand complexes.

Unit II Coordination Chemistry III **(14 hrs.)**

Kinetic stability, lability and inertness; ligand substitution reactions in octahedral and square planar complexes: acid hydrolysis, base hydrolysis and anation reactions; trans effect – theories and applications; electron transfer reactions: complementary and non-complementary types; inner and outer-sphere processes – applications of electron transfer reactions in synthesis of coordination complexes – reactions of coordinated ligand : mechanism of ascorbic acid oxidation by free and chelate Cu(II) Complexes.

Unit III NMR & EPR Spectroscopy **(10 hrs.)**

NMR: Applications of chemical shift and spin – spin coupling to structure determination using multiprobe NMR (B^{11}, F^{19} and P^{31}); effect of quadrupole nuclei on spectra; NMR studies on exchange rates and fluxional behavior; paramagnetic NMR and contact shifts.

EPR: Zero field splitting and Kramer's degeneracy; covalency of M-L bonding by EPR; EPR studies on Jahn Teller distortion in Cu(II) complexes; structural elucidation of inorganic compounds by EPR data.

Unit IV Solid state chemistry **(14 hrs.)**

Crystal defects : point, line and plane defects - intrinsic point defects: Schottky and Frenkel defects - extrinsic point defects: non-stoichiometric defect - preparation and physical properties of non-stoichiometric compounds, colour center.

Electronic structure of solids: free electron and band theories - types of solids: insulators. intrinsic and extrinsic semiconductors - optical and electrical properties of semiconductors: photovoltaic and Hall effect; superconductor, high T_c superconductors

– properties and applications, BCS theory; solid electrolytes: β-alumina and silver compounds and their applications.

Unique nature of solid state reactions and their different types with one example for each.

Unit V Inorganic Photochemistry (12 hrs.)

Properties of excited states, electronically excited states of metal complexes and charge transfer excitations - bimolecular deactivation and energy transfer processes; ligand field photochemistry – photosubstitution, photoisomerisation and photoredox reactions; synthesis, properties and charge transfer photochemistry of $Ru(bpy)_3^{2+}$ - photochemical conversion and storage of solar energy - photochemistry at semiconductor electrodes –Honda cell and water photolysis.

References:

1. D.F. Shriver, P.W. Atkins and C.H. Longford, Inorganic Chemistry, Oxford, 1990.
2. W.L.Jolly, Modern Inorganic Chemistry, McGraw Hill Company, 2nd Edn. 1991.
3. J.E. Huheey, E.A. Keiter and R.L. Keiter, Inorganic Chemistry, Harper and Row/Pearson Asia, 2,3 & 4th Edn.1993.
4. F.A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, John Wiley & Sons, 3,4&5th Edn.1988.
5. B.E. Douglas, D.H. McDaniel and J.J. Alexander, Concepts and Models of Inorganic Chemistry, John Wiley & Sons, 2nd Edn. 1983.
6. J.D. Lee, Concise Inorganic Chemistry, ELBS 1990.
7. R.F. Purcell and J. Kotz, Advanced Inorganic Chemistry, Saunders Golden.
8. R.S. Drago, Physical Methods in Chemistry, W.B. Saunders, 1997.
9. E.A. V. Ebsworth et al., Structural Methods in Inorganic Chemistry, ELBS 1987.
10. Azaraff, Introduction to Solids, Tata McGraw Hill, 11th Reprint, 1992.
11. 2. C.Kittel, Introduction to Solid State Physics, Wiley Eastern, 5th Edn. 1992.
12. 3. A. R. West, Solid state chemistry and its applications, John Wiley & Sons, New York, 2004.
13. J.K. Rohatgi – Mukherjee, Fundamentals of Photochemistry, Wiley Eastern Revised Edn.
14. J. Chem. Ed., October 1983 issue, American Chemical Society
15. A.W. Anderson and F.D. Fleischer, Concepts of Inorganic Photochemistry, John Wiley and Sons, New York, 1975.

PHYSICAL CHEMISTRY-II

Quantum Chemistry, Thermodynamics and Surface Chemistry

MCHC23		
L (hrs)	Credits	Course
60	4	Core

Unit I Quantum Chemistry I **(12 hrs.)**

Planck's Quantum theory – Wave particle duality – uncertainity principle, operators and commutation relation, postulates of quantum mechanics – simples systems – one dimensional box, three dimensional box – rigid rotator – harmonic oscillator – hydrogen atom, shapes of atomic orbitals – orbital and spin angular momenta.

Unit II Quantum Chemistry-II **(14 hrs.)**

Many electron systems – Pauli's antisymmetry principle – slater determinant – Approximation methods – variation and perturbation – applications to helium atom – Hartree Self Consistent field theory. Spin-orbit interaction –term symbols – vector model of the atom

Born-oppenheimer approximation – LCAO – MO for H_2^+ ion – VB treatment of H_2 molecule. Homo and heteronuclear diatomic - Hybridisation – sp, sp^2, sp^3, HMO theory – ethylene and butadiene.

Unit III Thermodynamics- II **(14hrs.)**

Ensemble of systems – state of a system – phase space – statistical equilibrium-microcanonical, canonical and grand canonical ensemble – micro and macro states; derivation of classical Boltzman distribution law; quantum statistics – Bose-Einstein, Fermi-Dirac and Maxwell-Boltzmann statistics – comparison of B. E. and F. D. statistics with Boltlzman statistics – photon gas and electron gas; Boltzmann-Planck equation; partition function – partition function and thermodynamics properties – partition function and equilibrium constant; concept of negative Kelvin temperature.

Unit VI Surface Chemistry -I **(10 hrs.)**

Liquid interfaces – Gibbs adsorption isotherm – surface films – spreading of one liquid on another – measurement of film pressure;; solid-liquid interfaces – contact angle – wetting as a contact angle phenomenon – wetting as a capillary action phenomenon; detergency – general aspects of soil removal – factors in detergent action; foams and aerosols.

Unit V Surface Chemistry –II **(10 hrs.)**

Solid-gas interfaces – physisorption , chemisorptions –Langmuir, Freundlich and BET isotherms - surface area determination – heats of adsorption; heterogeneous catalysis – role of surfaces in catalysis – semiconductor catalysis – n-and p-type surfaces; kinetics of surface reactions involving adsorbed species – Langmuir- Hinshelwood mechanism – Langmuir – Rideal mechanism.

References:

1. A.K. Chandra, Introduction to quantum Chemistry, Tata McGraw Hill, New Delhi, 1997.
2. L.N. Levine, Quantum Chemistry, Prentice Hall, New Delhi 1994
3. R.K. Prasad Quantum Chemistry, Wiley Eastern, 1993
4. F.E. Pilar, Elementary Quantum Chemistry, McGraw-Hill, New Delhi, 1968
5. S. Glasstone, Theoretical Chemistry, Van Nostrand, New York, 1944
6. S. Glasstone, Thermodynamics for chemists, Van Nostrand, New York, 1969.
7. M. C. Gupta, Statistical Thermodynamics, Wiley-Eastern, New Delhi, 1990.
8. J. Rajaram, J.C. Kuriacose, Thermodynamics for chemistry, Shoban Lal Nagain Chand, New Delhi, 1986.
9. A.W. Adamson, Physical Chemistry of Surfaces, 5th Edition, John Wiley and Sons, New York, 1990.
10. S. Glasstone, Text Book of Physical Chemistry, 2nd Edition, Macmillan India Ltd, New Delhi , 1974.
11. K.J. Laidler, Chemical Kinetics, 2nd Edition, Tata McGraw –Hill, New Delhi 1991.
12. J.C. Kuriacose, Catalysis, Macmillan India Ltd., New Delhi, 1991.

PRACTICALS

ORGANIC CHEMISTRY PRACTICAL – II

MCHL21		
L (hrs)	Credits	Course
60	2	Practical

1. Separation and systematic analysis of Organic binary mixtures.
2. Estimation of phenol, aniline, methyl ethyl ketone, glucose.

References

1. A. I. Vogel, A Text Book of Practical Organic Chemistry.
2. A. Ault, Techniques and Experiments for Organic Chemistry.
3. N. K. Vishnoi, Advanced Practical Organic Chemistry.
4. B. B. Dey and M.V. Sitaraman, Laboratory Manual of Organic Chemistry.
5. Raj K. Bansal, Laboratory Manual in Organic Chemistry.

INORGANIC CHEMISTRY PRACTICAL – II

MCHL22		
L (hrs)	Credits	Course
60	2	Practical

1. Separation and estimation of metal ions in a mixture by volumetric and gravimetric methods. Some typical recommended mixtures are: Cu(II) & Ni(II); Fe(II) & Cu(II); Cu(II) & Zn(II); Ca(II) & Ba(II); Fe(II) & Ni(II); Cu(II) & Ca(II)

References:

1. 'Vogel's Text Book of Quantitative Chemical Analysis', Eds. G.H. Jeffrey, J.Banett, J. Mendham and R.C. Denney, ELBS, 5th Edn. Reprint 1991.

SEMESTER III

ORGANIC CHEMISTRY – III

MCHC31		
L (hrs)	Credits	Course
60	4	Core

Unit I **(12 hrs.)**

a) UV Spectroscopy

Various electronic transitions (185–800 nm), Beer–Lamberts law, effect of solvent on electronic transitions, ultraviolet bands for saturated and unsaturated carbonyl compounds, dienes, conjugated polyenes. Fieser–Woodward rules for conjugated dienes and carbonyl compounds, ultraviolet spectra of aromatic and heterocyclic compounds – Scott's rules – shift reagents – steric effect in biphenyls.

b) IR Spectroscopy

Instrumentation and sample handling – characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols and amines. Detailed study of vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters, amides, acids, anhydrides, lactones, lactams, and conjugated carbonyl compounds). Effect of hydrogen bonding and solvent effect on vibrational frequencies, overtones, combination bands and Fermi resonance, FT–IR.

Unit II **(12 hrs.)**

a) ^{1}H, ^{13}C–NMR Spectroscopy

General introduction and definition, chemical shift, spin-spin interaction, shielding mechanism, mechanism of measurement, chemical shift values and correlation for protons bonded to carbon–(aliphatic, olefinic, acetylenic, aromatic) and other nuclei (alcohols, phenols, enols, carboxylic acids, amines, amides and mercaptans), chemical exchange, virtual coupling. Stereochemistry, hindered rotation, Karplus curve – variation of coupling constant with dihedral angle. Simplification of complex spectra – double resonance, shift reagents, NOE, FT–technique – Spin Relaxation

General considerations ^{13}C–NMR Spectroscopy – chemical shift (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbon), coupling constants. 2-D NMR–COSY, DEPT.

b) Mass spectrometry

Introduction to EI. Factors affecting fragmentation. Mass spectral fragmentation of organic compounds containing common functional groups, molecular ion peak,

nitrogen rule, metastable peak, McLafferty rearrangement – Isotopic peaks, CI, FAB, MALDI.

c) Combined Spectral Problems:

Spectral problems involving UV, IR, NMR and Mass spectral data.

Unit III Retro Synthetic Analysis: (12 hrs.)

Strategy and planning-starting material-Linear and Convergent approach, protecting groups and activating groups. Regioselectivity, chemoselectivity. diastereoselectivity. Target molecules containing one functional group requiring a single disconnection- Synthons and synthetic equivalents. Latent polarity. Target molecules with two functional groups– 1,2-, 1,3-, 1,4-, 1,5-, and 1,6-dicarbonyl compounds, Umpolung reactions. Functional group interconversions. Retrosynthetic analysis of 2,4–dimethyl–2–hydroxypentanoic acid, trans-9-methyl–1–decalone, α-onocerin, β-bisabolene.

Unit IV Supramolecular Chemistry: (10 hrs.)

Definition – host-guest chemistry – classification of supramolecular host-guest compounds – coordination and the lock and key analysis – the chelate, macrocyclic and template effects – nature of supramolecular interactions – spherands, lariat ethers, podants, cryptands – molecular recognition, chiral recognition, molecular sieves, molecular wires, molecular switches.

Unit V Reaction mechanism (14 hrs.)

a)Selected name reactions: Aldol, Dieckmann condensation, Reformatsky, Wittig and Mannich reaction, Oppenauer oxidation, Clemmenson, Wolff-Kishner, Meerwin-Pondorf-Verley (MPV) and Birch reductions, McMurry and Polonovski reaction.

b) Reagents in Organic Synthesis

Complex metal hydrides, Gilman reagent (lithium dialkylcuprates), lithium diisopropylamide (LDA), dicyclohexylcarbodiimide(DCC), Woodward and Prevost hydroxylation, DDQ, selenium dioxide, Phase Transfer Catalyst (PTC), Wilkinson catalyst, crown ethers, Peterson's synthesis.

INORGANIC CHEMISTRY - III

MCHC32		
L (hrs)	Credits	Course
60	4	Core

Unit I Organometallic Chemistry I **(12 hrs.)**

EAN rule and its correlation to stability of organometallic compounds - synthesis, structure and bonding of metal carbonyls, nitrosyls and dinitrogen complexes; IR spectral characterization of carbonyls and nitrosyls - pi – acceptor complexes with alkene, alkyne, allyl and arene systems – Metallocenes; synthesis, properties, structure and bonding with particular reference to ferrocene and berryllocene.

Unit II Organometallic Chemistry II **(14 hrs.)**

Substitution reactions of carbonyls; oxidative addition and reductive elimination, insertion and elimination reactions; nucleophilic and electrophilic attack of coordinated ligands; addition to bimetalic species and cyclometallation reactions.

Homogeneous catalysis – organometallic compounds functioning as catalysts and the requirements; Wilkinson's catalyst and hydrogenation reactions, Tolman's catalytic loop; hydroformylation (oxo) reaction, Wacker and Monsanto acetic acid processes. Cluster compound, polymer-supported and phase-transfer catalysis.

Heterogeneous catalysis – synthesis gas and water gas shift reactions; Fischer Tropsch process and synthetic gasoline, Ziegler-Natta polymerization and mechanism of stereoregular polymer synthesis.

Unit III Mossbauer spectroscopy & Analytical Techniques **(10 hrs.)**

Mossbauer spectroscopy: principle, isomer shift, quadruple and magnetic interactions. Mossbauer studies of octahedral high and low spin Fe(II) and Fe(III) complexes; information on oxidation state, π-back coordination, structure and nephelauxetic effect in iron compounds; studies on halides of tin(II) and tin(IV) compounds.

Spectroanalytical techniques: Spectrophotometry, fluorimetry, nephelometry, and turbidimetry.

Electroanalytical techniques: Cyclic voltammetry, stripping voltammetry and amperometric titrations.

Unit IV Bioinorganic Chemistry I **(12 hrs.)**

Non-metals and metals in biological systems, essential and trace elements; classification of metallo-biomolecules, coordination environment and entatic state.

Porphyrin – metal complex systems – chlorophyll and photosynthesis; cytochromes, hemoglobin, myoglobin and dioxygen binding, vitamin B_{12} and co-enzyme - *in vivo* and *in vitro* nitrogen fixation.

Iron storage and transport : ferritin, transferrins and siderophores - iron proteins: hemerythrin, cytochrome P450 enzyme, ferredoxin and rubredoxin.

Unit V – Bioinorganic Chemistry II (12 hrs.)

Copper proteins and Enzymes : plastocyanin, azurin, hemocyanin and ascorbic oxidase - different types of Cu present in proteins and enzymes.

Zinc enzymes : carboxypeptidase A, carbonic anhydrase and superoxide dismutase.

Inhibition and poisoning of enzymes illustrated by xanthine oxidase and aldehyde oxidase.

Toxicity of metals and the role of metallothionins - excess and deficient levels of Cu,and Fe and the consequent diseases - chelate therapy – metal complexes as drugs, anticancer and antiarthritic agents. Metal complexes as probes of nucleic acids.

References

1. D.F. Shriver, P.W. Atkins and C.H. Longford, Inorganic Chemistry, Oxford, 1990.
2. W.L. Jolly, Modern Inorganic Chemistry, McGraw Hill Company, 2nd Edn. 1991.
3. J.E. Huheey, E.A.Keiter and R.L. Keiter, Inorganic Chemistry, Harper and Row/Pearson Asia, ,3 & 4th Edn. 1993.
4. F.A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, John Wiley & Sons, 3,4 & 5th Edn. 1988.
5. B.E. Douglas, D.H. McDaniel and J.J. Alexander, Concepts and Models of Inorganic Chemistry, John Wiley & Sons, 2 Edn. 1983.
6. H.H. Willard, L.L.Merritt, J.A.Dean and F.A. Settle, Instrumental methods of Analysis 6th
7. Edn. CBS publishers, 1986.
8. 'Vogel's Text Book of Quantitative Chemical Analysis' Edn. G.H. Jeffrey, J.Banett, J.Mendham and R.C. Denney, ELBS, 5th Edn.1989.
9. D.A. Skoog and D.M. West, Principles of Instrumental Analysis, HoltSaunders, 2 Edn. 1980.
10. D.A. Skoog and J.J. Leary, Instrumental Analysis, Saunders College publishing, 1992.
11. D. Banerjea, Coordination Chemistry, Tata McGraw Hill, 1933.
12. A.K. Das, Bioinorganic Chemistry, Books and Allied (P) Ltd., Reprint 2012

MCHC33		
L (hrs)	Credits	Course
60	4	Core

PHYSICAL CHEMISTRY – III

Group Theory, Molecular Spectroscopy and Polymer Chemistry

Unit I Group Theory-I (10 hrs.)

Elements of group theory – properties of group – subgroups and classes; symmetry elements and symmetry operations – symmetry point groups; matrix algebra—matrix representation of geometric transformation – reducible and irreducible representation; Great orthogonality theorem – construction of character tables; direct products.

Unit II Group Theory-II (14 hrs.)

Application of group theory to normal mode analysis –symmetry selection rules for IR and Raman active fundamentals; symmetry of molecular orbitals and symmetry selection rule for electronic transitions in simple molecules (ethylene, formaldehyde and benzene); projection operators – SALC procedure – evaluation of energies and MO's for ethylene, butadiene and cyclopropenyl systems – application of group theory to solve hybridization problems.

Unit III Molecular Spectroscopy-I (12 hrs.)

Characterization of electromagnetic radiation - signal to noise ratio – the width and intensity of spectral transitions; microwave spectroscopy – rotational spectra of diatomic and simple polyatomic molecules; infrared spectroscopy – harmonic and anharmonic oscillator – vibration – rotation spectra of diatomic and polyatomic molecules- influence of rotation on the spectra of polyatomic molecules – parallel and perpendicular vibrations.

Raman spectroscopy – theory of Raman effect – pure rotational Raman spectra - vibrational Raman spectra –mutual exclusion principle

Unit IV Molecular spectroscopy-II (14 hrs.)

Electronic spectroscopy – Born- Oppenheimer approximation – vibrational coarse structure – Franck-Condon principle – dissociation energy – rotational fine structure of electronic – vibration transitions- Fortrat diagram – predissociation.

Photoelectron spectroscopy – basic principles – Auger transitions – valance and core binding energy analysis – ESCA.

NMR Spectroscopy – spin and an applied field – nature of spinning particles – interaction of spin magnetic field – population of energy levels; chemical shift and coupling constant

NQR spectroscopy – principles- experimental set up- nuclear quadrupole coupling in atoms and molecules – applications; ESR spectroscopy – basis principles – hyperfine splitting – origin of hyperfine interaction – the g value – Mc Connel relationship – applications of ESR.

Unit V Photochemistry **(10 hrs.)**

Photophysical processes in electronically excited molecules – fluorescence phosphorescence, delayed emission and other deactivation process – Stern – Volmer equation and its applications – Photosensitization – conventional photolysis procedure – flash photolysis, elementary aspects of photosynthesis, phototochemical chain reactions – H_2 – Br_2 reaction – ozone depletion – photochemical conversion and storage of solar energy.

References

1. F. A. Cotton, Chemical Applications of Group Theory, Wiley-Eastern, New Delhi, 1971.
2. G. Davidson, Introductory Group Theory for Chemists, Applied Science Publishers, London, 1971.
3. V. Ramakrishnan and M. S. Gopinathan, Group theory and Chemistry, Vishal Publications, Delhi, 1991.
4. K.V. Raman, Group theory and its Applications to Chemistry, Tata McGraw-Hill, New Delhi, 1990.
5. D. C. Harris, M.D. Bertolucci, Symmetry and Spectroscopy, Oxford University Press, New York, 1978.
6. R. S. Drago, Physical Methods in Chemistry, Saunders, London, 1977.
7. C.N. Banwell, Fundamentals of Molecular Spectroscopy, Tata McGraw-Hill, New Delhi, 1990.
8. R. Chang, Basic Principles of Spectroscopy, McGraw-Hill, New Delhi, 1971.
9. G. M. Barrow, Introduction to Molecular Spectroscopy, Tata McGraw-Hill, New Delhi, 1964.
10. B.P. Straughan and S. Walker, Spectroscopy, Vol. 1, 2 & 3, Chapman and Hall, London, 1976.
11. C. D. Becker, High Resolution NMR – Theory and Applications, Academic Press, New York, 1980.
12. D. W. Claridge, High Resolution NMR Techniques in Organic Chemistry, Pergamon, 1999.

13. K.K. Rohatgi – Mukerjee, Fundamentals of Photochemistry, Wiley – Eastern, New Delhi, 1978.
14. J.R. Lakowicz, Principles of fluorescence spectroscopy, Plenum Press, New York 1999.
15. N.S. Turro, Molecular Photochemistry, Benjamin, 1965
16. J.G. Calvert J.N. Pitts, Photochemistry, Wiley, Newyork, 1966

PAPER - RESEARCH METHODOLOGY

MCHP31		
L (hrs)	Credits	Course
60	4	Core

Literature Survey And Research Methodology

Literature Survey and Research Methodology (Seminar paper related to project work in IV semester). This paper in III Semester forms the foundation for Project work in IV Semester*. Hence the students are allotted in the beginning of III Semester itself to the Teacher/Guide for their project work in IV Semester.*

Unit I **(15 hrs.)**

Introduction to research, selection of a research topic, reviewing the literature, preparing the proposal and design of study. Experimentation and interpretation of results. Formation, testing and rejection of hypothesis. Application of microcal origin and chemdraw. Preparation and presentation of report; dissertation and thesis writing.

Primary and secondary literature: Journals, patents, Reviews, Chemical abstracts, treatises and monographs. Printed materials and online literature search; websites, search engine for locating information and chemical data bases. E-mail operation and online submission of manuscripts for publication.

Unit II **(10 hrs.)**

Limitations of analytical methods; accuracy, precision and minimization of errors. Systematic and random errors and reliability of results. Replicate determination and t-test. Correlation, linear regression and analysis of variance.

Unit III **(10 hrs.)**

Principles, sampling techniques and application of UV VIS spectrophotometry, far, near and FTIR spectrophotometry and ICP spectrometry. Thermo analytical techniques: TGA, DTA, DSC and thermometric titrations. Magnetic susceptibility and EPR spectroscopy measurements and characterization of samples.

Units IV & V **(25 hrs.)**

Syllabus for these two units (published papers in journals) shall be provided to the students by the concerned Teacher/guide to whom the students are allotted in the III Semester itself for their project work in the IV Semester.

References:

1. Rajammal P. Devadas, A Handbook of Methodology of Research, S.R.K. Vidyalaya Press, Chennai, 1976.
2. J. Anderson, B.H. Durstan and M. Poole, Thesis and assignment writing, Wiley Eastern, New Delhi, 1977.
3. R.O. Butlet, Preparing thesis and other manuscript.
4. Jerry March, Advanced Organic Chemistry, 4th Edn. John Wiley & Sons, 1992.
5. V ogel's Textbook of Quantitative Chemical Analysis, 5th Edn. ELBS, 1978.
6. H.H. Willard, L.L. Merritt, J.A. Dean and F.A..Settle, Instrumental Methods of Chemical Analysis, 6th Edn. CBS Publishers, New Delhi, 1986.
7. Chromatographic Methods – R. Stock and B.R. Rice (Chapman & Hall 1974)
8. Reaction Mechanism and Reagents in Organic Chemistry – Gurdeep R. Chatwal
9. A.J. Bard and L.R. Faulkner, Electrochemical Methods : Fundamentals and Applications, 2nd Edn., John Wiley and Sons, New York, 2004.
10. L. Antropov, Theoretical Electrochemistry, Mir Publication, Moscow, 1972.
11. D.A. Skoog and J.J. Leary, Principles of Instrumental Analysis, 4th Edn., Saunders College Publishing, 1992.
12. D.A. Skoog, F.S.Holler, S.R.Crouch, Principles of Instrumental Analysis, 6th Edn., Thomson Brooks/cole, 2007.
13. A.K. Cheetham, P.Day, Solid State Chemistry: Techniques, Oxford University Press, Oxford, 1987.
14. G. E. Bacon, Neutron diffraction, Oxford Universtiy Press, Oxford, 1975.
15. R.S. Drago, Physical Methods in Chemistry, Saunders, 1999.

PHYSICAL CHEMISTRY PRACTICAL – I

MCHL31		
L (hrs)	Credits	Course
60	2	Practical

Part 1: Conductivity

a. Determination of cell constant
b. Dissociation constant of a weak acid
c. Conductometric titrations:
   i) Estimation of HCl and AcOH in a mixture
   ii) Estimation of NH_4Cl and HCl in a mixture
   iii) Estimation of AcOH and Sodium acetate in a buffer
   iv) $BaCl_2$ *vs* $NaCO_3$

Part 2: Distribution law

a. Partition coefficient of Iodine between two immiscible solvents.
b. Study of the equilibrium constant of the reaction $KI + I_2 = I_3$. KI/3

Part 3: Kinetics (atleast one)

1. Acid hydrolysis of ester – comparison of strength of acids.
2. Kinetics – persulfate – Iodide – clock reaction-primary salt effect.

References:

1. W. J. Popiel, Laboratory Manual of Physical Chemistry, ELBS, London 1970
2. Findlay's Practical Physical Chemistry, B. P. Levitt, Longman, London, 1985
3. S. K. Sinha, Physical Chemistry A Laboratory Manual, Narosa Publishing Pvt, Ltd., 2014.

PHYSICAL CHEMISTRY PRACTICAL – II

MCHL32		
L (hrs)	Credits	Course
60	2	Practical

Part 1: Potentiometry

a. Determination of solubility product of sparingly soluble silver salts.
b. Determination of dissociation constant of weak acids.
c. Potentiometric titrations:
    i) Redox titrations
        a) Fe^{2+} vs $Cr_2O_7^{2-}$
        b) Fe^{2+} vs Ce^{4+}
        c) I^- vs $KMnO_4$
    ii) Precipitation titration
        a) Cl^- vs Ag^+
        b) I^- vs Ag^+
        c) Mixture of Cl^- and I^- vs Ag^+

Part 2: Adsorption of oxalic acid/acetic acid on charcoal.

Part 3: Titration using pH meter – determination of dissociation constant of dibasic acid (Demonstration).

References:

1. W. J. Popiel, Laboratory Manual of Physical Chemistry, ELBS, London 1970
2. Findlay's Practical Physical Chemistry, B. P. Levitt, Longman, London, 1985
3. S. K. Sinha, Physical Chemistry A Laboratory Manual, Narosa Publishing Pvt, Ltd., 2014.

SEMESTER IV

MCHOEA		
L (hrs)	Credits	Course
45	3	Elective

ELECTIVE PAPER – I - ORGANIC

Advanced Organic Chemistry

Unit I Photochemistry **(11 hrs.)**

Photophysical processes - Jablonski diagram - Photochemical intramolecular reactions of the olefinic bond, geometrical isomerism, cyclization reactions, rearrangement of 1,3- and 1,5-dienes.

Intramolecular reactions of carbonyl compounds: Structural, cyclic and acyclic, Norrish type I and II, α, β-unsaturated and β, γ-unsaturated compounds – cyclohexadienones.

Intermolecular reactions of carbonyl compounds-cycloaddition reaction, dimerizations, Paterno-Buchi reaction.

Photosensitization, photo-oxidation, auto-oxidation, photo-reduction, Barton reaction, photo-Fries rearrangement, di-π-methane rearrangement. Photo chemistry of vision.

Unit II **(11 hrs.)**

a) **Pericyclic reactions** - conservation of molecular orbital symmetry - electrocyclic and cycloaddition reactions - Sigmatropic rearrangements - applications of correlation diagram - Applications of Frontier Molecular Orbital (FMO) theory. Perturbation Molecular Orbital (PMO) theory and Huckel-Mobius approach to the above reactions – Hofmann-Loffler-Freytag reactions, Ene synthesis, cheletropic reactions.

b) Molecular Rearrangements

Rearrangement to electron-deficient carbon: Wagner-Meerwin, benzil-benzilic acid.

Rearrangement to electron-deficient nitrogen: Hofmann, Curtius, Beckmann

Rearrangement to electron-deficient oxygen: Baeyer-Villiger

Rearrangement proceeding through electron-rich carbon: Sommelet-Hauser, Favorskii.

Unit III **(09 hrs.)**

a) **Heterocycles**

General methods of synthesis and reactions of carbazoles, acridines, oxazoles, isoxazoles, thiazoles, isothiazoles, pyridazine, pyrimidine Synthesis and applications of polypyrrole and polythiophene.

b) Alkaloids and Terpenoids:

Alkaloids: Classification –Biosynthesis of alkaloids and terpenoids – structural elucidation of α-pinene

Unit IV Antibiotics, Vitamins and Steroids (07 hrs.)

Vitamins: A_1, A_2, B_1, B_2, C, H.

Antibiotics: chloramphenicol, cephalosporin.

Steroids: Androsterone, testosterone, estrone, progesterone.

Unit V Catalysis and Green Chemistry (07 hrs.)

Introduction, basic principles of green chemistry. Designing a green synthesis: Green starting materials, green reagents, green solvents and reaction conditions, green catalysts. Use of the following in green synthesis with suitable examples. Green reagents: dimethylcarbonate, polymer supported reagents. Green catalysts: Acid catalysts, oxidation catalysts, basic catalysts, phase transfer catalysts and biocatalysts. Green solvents: water, ionic liquids, deep eutectic solvents, supercritical carbon dioxide. Solid state reactions: solid phase synthesis, solid supported synthesis. Microwave assisted synthesis: reactions in water, reactions in organic solvents, solvent free reactions. Ultrasound assisted reactions.

ELECTIVE PAPER II - ORGANIC

Pharmaceutical Chemistry

MCHOEB		
L (hrs)	Credits	Course
45	3	Elective

Unit I **(09 hrs.)**

Introduction to the history of pharmaceutical chemistry, general mechanisms of drug action on lipids, carbohydrates, proteins and nucleic acids, drug metabolism and inactivation, receptor structure and sites, drug discovery development, design and delivery systems, gene therapy and drug resistance.

Unit II **(09 hrs.)**

Classification of drugs based on structure and pharmacological basis with examples. Synthesis of important drugs such as α-methyl dopa, Chloramphenicol, griseofulving, cephelosphorins and nystatin. Molecular modeling, conformational analysis, qualitative and quantitative structure activity relationships.

Unit III **(10 hrs.)**

General introduction to antibiotics, mechanism of action of lactam antibiotics and anon lactam antibiotics, antiviral agents, chemistry, stereochemistry, biosynthesis and degradation of penicillins – An account of semisynthetic pencillins – acid resistant, pencillinase resistant and broad spectrum semisynthetic pencillins.

Unit VI **(08 hrs.)**

Elucidation of enzyme structure and mechanism, kinetic, spectroscopic, isotopic and stereochemical studies. Chemical models and mimics for enzymes.

Design, synthesis and evaluation of enzyme inhibitors.

Unit V **(09 hrs.)**

DNA-protein interaction and DNA-drug interaction. Introduction to rational approach to drug design, physical and chemical factors associated with biological activities, mechanism of drug action.

ELECTIVE PAPER – III - ORGANIC

Bio-organic Chemistry

MCHOEC		
L (hrs)	Credits	Course
45	3	Elective

Unit I Carbohydrate **(09 hrs.)**

Glycolysis, various forms of fermentations in micro-organisms, citric acid cycle, its function in energy generation and biosynthesis of energy rich bond, pentose phosphate pathway and its regulation. Gluconeogenesis, glycogenesis and glycogenolysis, glyoxylate and Gamma aminobutyrate shunt pathways.

Unit II Amino Acids **(09 hrs.)**

General reactions of amino acid metabolism - Transamination, decarboxylation, oxidative & non-oxidative deamination of amino acids. Special metabolism of methionine, histidine, phenylalanine, tyrosine, tryptophan, lysine, valine, leucine, isoleucine and polyamines. Urea cycle and its regulation.

Unit III Lipids **(09 hrs.)**

Introduction, hydrolysis of tri-acylglycerols, α-, β-, ω- oxidation of fatty acids. Oxidation of odd numbered fatty acids – fate of propionate, role of carnitine, degradation of complex lipids. Fatty acid biosynthesis, Acetyl CoA carboxylase, fatty acid synthase, ACP structure and function Lipid biosynthesis, biosynthetic pathway for tri-acylglycerols, phosphoglycerides, sphingomyelin and prostaglandins. Metabolism of cholesterol and its regulation. Energetics of fatty acid cycle.

Unit IV Nucleotides **(09 hrs.)**

Biosynthesis and degradation of purine and pyrimidine nucleotides and its regulation. Purine salvage pathway. Role of ribonucleotide reductase. Biosynthesis of deoxyribonucleotides and polynucleotides including inhibitors of nucleic acid biosynthesis.

Unit V: **(09 hrs.)**

a) **Porphyrins –** Biosynthesis and degradation of porphyrins. Production of bile pigments
b) **Biosynthesis of Vitamins –** Ascorbic acid, thiamine, pantothenic acid and Folic acid.

References for Organic Chemistry Theory papers: (IV Semesters)

1. Peter Sykes, A Guidebook to Mechanism in Organic Chemistry, Orient Longman, New Delhi, 1989.
2. J. Clayden, N. Greeves, S. Warren and P. Wothers, Organic Chemistry, Oxford University Press Inc., New York, 2001.
3. Jerry March, Advanced Organic Chemistry, 4th edition, John Wiley & Sons Inc., New York, 1992.
4. S.M. Mukherji and S.P Singh, Reaction Mechanisms in Organic Chemistry, Macmillan India Ltd., New Delhi, 1997.
5. E.S. Gould, Mechanism and Structure in Organic Chemistry, Henry Holt, Reinhart and Winston Inc, New York, 1959.
6. T.W.G Solomon, Organic Chemistry, 5th edition, John Wiley & Sons, Inc., New York, 1992.
7. F.A Carey and R.J. Sundberg, Advanced Organic Chemistry, part A & B 3rd Edn. Plenum Press, New York, 1993.
8. R.O.C Norman and J.M. Coxon, Principles of Organic Synthesis, 3rd Ed. ELBS with Chapman & Hall, 1993.
9. Streitweiser and C.H. Heathcock, Introduction to Organic Chemistry, Macmillan ublishing Co., Inc., New York, 1976.
10. G.M. Badger Aromatic Character and Aromaticity, Cambridge, 1969.
11. P.J. Garratt, Aromaticity, McGraw-Hill Book Co., New York, 1971.
12. T.H. Lowry and K.S. Richardson, Mechanism and Theory in Organic Chemistry.
13. V.K. Ahluwalia and R.K. Parashar, Organic Reaction Mechanisms, Narosa Publishing House, 2002.
14. R.T. Morrison and R.N. Boyd, Organic Chemistry, Prentice Hall, 1992.
15. D.J Ager, Handbook of Chiral Chemicals, Marcel Dekker, Inc.,New York 1999.
16. V.M. Potapov, Stereochemistry, MIR Publishers, Moscow, 1979.
17. E.L. Eliel and S.H Wilen, Stereochemistry of Organic Compounds, John Wiley & Sons, Inc. 1994.
18. E.L. Eliel, Stereochemistry of Carbon Compounds, 24th reprint, Tata McGaw-Hill Publishing Company Ltd., New Delhi,1999.
19. D. Nasipuri, Stereochemistry of Organic Compounds, Principles and Applications, New Age International (P) Ltd., New Delhi 2000(Second Edition).

20. J.A Joule and K. Mills, Heterocyclic Chemistry, 4th Edition, Blackwell Science Ltd., Edinburgh, U.K.
21. I.L. Finar, Organic Chemistry, Vol-I & Vol-II, 5th Edition 1975, Pearson Education Asia Pte. Ltd., Ist Indian Reprint, 2000.
22. R.K. Bansal, Heterocyclic Chemistry, Wiley Eastern Ltd., New Delhi, 1990.
23. R.M. Acheson, An Introduction to the Chemistry of Heterocyclic Compounds, Wiley Eastern Ltd., New Delhi.
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26. Bentley, The Alkaloids, Interscience Publishers 1957
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28. G. Zubay, Biochemistry, Addison–Wesley Publishing Company Ltd.,1983.
29. G. R. Chatwal, Organic Chemistry of Natural Products, Himalaya Publishing House, New Delhi, 1985.
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36. P.R.Young, Practical Spectroscopy, The Rapid Interpretation of Spectral Data Brooks/Cole, California, 2000.
37. R. Davis, M. Frearson, Mass Spectrometry, John Wiley & Sons, New York, 1991
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40. R.E. Ireland, Organic Synthesis, Prentice-Hall of India Pvt. Ltd, New Delhi,1975.
41. J.W. Steed and J.L. Atwood, Supramolecular Chemistry, John Wiley & Sons, New York.

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43. Vertos Chemis, The Conservation of Orbital Symmetry, Gmbh and Asadan Press, 1971.
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45. Jagdamba Singh and Jaya Singh, Photo Chemistry and Pericyclic Reaction, New Age International (P) Ltd., New Delhi, 2003.
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51. L.S. Hegedus, Transition metals in the synthesis of complex organic molecules, University Science Books, Mill Valley, California, 1994.
52. Supramolecular Chemistry – Steed and Alkins – Jonh Wiley & Sons Ltd.,
53. Name Reactions – JieJackli – 2nd Edn. Springer
54. Organic Structure Determination – D.J. Pasto and ER. Johnson – Prentice-Hall, Inc., 1969.
55. Rashmi Sanshi, M.M. Srivastra – Green Chemistry – Alpha Sciences, 2003.
56. V. Murugesan et al Recent trends in catalysis. Narosa publications. 1998.
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58. J. Ghosh, Fundamental Concepts of Applied Chemistry, S. Chand and Co., New Delhi, 2006; A.Kar, Medicinal Chemistry, New Age International (P) Ltd, Delhi, 1997.
59. Principles of Biochemistry - L. Stryer (W.H. Freeman & Co.)
60. Principles of Biochemistry - A.L.Lehninger, D.W.Nelson & M.M.Cox (Macmillan)
61. Biochemistry - D.Voet & J.G.Voet (John Willey).
62. Harper's Illustrated Biochemistry - R.K.Murray et al. (McGraw Hill).

63. Lehninger's Principle of Biochemistry by David L. Nelson and Michael M. Cox. W. H. Freeman; 4th edition (2004).
64. Text Book of Biochemistry with clinical correlation by Thomas .M. Devlin, John Wiley-Liss, Hobokhen NJ publishers (2006).
65. Biochemistry by Zubey, GL WCB Publishers.

MCHIEA		
L (hrs)	Credits	Course
45	3	Elective

ELECTIVE PAPER I – INORGANIC

Instrumental Techniques for Materials Characterization

(Principle, Sample Preparation, Data acquisition and their analysis and one or two qualitative and quantitative applications; (No instrumentation part necessary).

Unit I Diffraction and Microscopic techniques (09 hrs.)

Classification and Review of instrumental techniques; materials characterization and a survey of available instrumental techniques.

Diffraction techniques: X-ray powder and crystal diffraction, electron microspcopy: SEM, TEM and AFM.

Unit II Spectroscopic Techniques I (10 hrs.)

Electromagnetic spectrum and the associated spectral techniques. Vibrational spectroscopy- IR & Raman; electronic spectroscopy – UV & visible; NMR & EPR spectroscopy.

Unit III Spectroscopic Techniques II (08 hrs.)

X-ray absorption and emission spectroscopy: XRF, photoelectron spectroscopy (XPS) and EXAFS. Atomic absorption spectroscopy (AAS): interferences in spectral observation and applications; inductively coupled plasma (ICP) sources.

Unit IV Thermal Analysis Techniques (08 hrs.)

General principles of various thermal analysis techniques – Differential scanning colorimetry (DSC) and differential analysis – Thermogravimetry (TGA) – evolved gas detection and analysis; Differential thermal analysis (DTA).

Unit V Mass spectrometry (10 hrs.)

Components of mass spectrometer – coupling or interfacing with other instruments. Inlet sample systems, ionization methods and mass analyzers. FT mass spectrometry, secondary ion mass spectrometry. Correlation of mass spectra with structure – General rules for prediction of mass spectra, Quantitative analysis of mixtures. Advantages of mass spectrometry over other methods.

References:

1. H.H. Willard, L.L. Merritt, J.A Dean and F.A. Settle, Instrumental Methods of Analysis , 7th Edn. CBS Publishers, First Indian Edn. 1986.

2. A.R. West, Solid state chemistry and its applications, Wiley, Reprint 2004.
3. D.A. Skoog, F.J. Holler, S.R. Crouch, Instrumental Analysis, Cengage Learning, 2007.
4. S.M. Khopkar, Basic Concepts of analytical Chemistry, 2nd Edn. New Age International, 1998.
5. G.H. Jeffery, J. Bassett, J. Mendham, R.C. Denney, Vogel's textbook of Quantitative Analysis5th Edn., ELBS reprint 1996.
6. H.R. Allcock, Introduction to Materials Chemistry, Wiley 2008.

ELECTIVE PAPER II-INORGANIC

Advanced Industrial Inorganic compounds

MCHIEB		
L (hrs)	Credits	Course
45	3	Elective

Unit I Ceramics (09 hrs.)

Ceramics – classification, optical waveguides (optical fiber), sol-gel formation for low temperature ceramic formation. Non-oxide ceramics – general aspects, silicon carbide, silicon nitride and boron nitride ceramics. Fabrication of ceramic materials and its challenges.

Unit II Carbon and other non-metal and metal fibers & zeolites (09 hrs.)

Carbon fibers: introduction, manufacture, applications and economic importance. SiC-coated carbon fibers. Aluminium oxide coated fibers; their manufacture and applications.

Zeolites: Natural and synthetic zeolites, manufacture of synthetic zeolites from different sources, pelletization, dehydration and applications.

Unit III Metal oxide pigments (09 hrs.)

Inorganic pigments: white pigments: TiO_2 pigment, its manufacture, post-treatment and applications; ZnO white, lithopone and ZnS pigments. Coloured pigments: iron oxide pigments – manufacture, oxidation processes and applications.

Unit IV Elemental Silicon & silicones (08 hrs.)

Silicon: metallurgical grade, ferrosilicon and electronic grade silicon, manufacture and applications.

Silicones & poly(organo siloxanes) (POS): manufacture, linear and branched POS, high molecular weight POS; silicone oil, emulsion, rubbers and resins.

Unit V Inorganic Polymers (10 hrs)

General characteristics, degree of polymerization, catenation and heterocatenation, S-N chain one dimensional conductor, isopoly and heteropoly acids (polyoxometallates) and their characteristics and applications (introductory level), phosphazene polymers; Metal clusters: dinuclear, trinuclear, tetranuclear and hexanuclear clusters and their synthesis and properties.

References

1. H.R. Allcock, Introduction to Materials Chemistry, Wiley, 2008.
2. S.K. Agarwala, Keemti Lal, Advanced Inorganic Chemistry, Pragati Prakashan, 10th edn., 2011.
3. A.R. West, Solid State Chemistry and its applications, Wiley, 2004.
4. M.G. Arora, M. Singh, Industrial Chemistry, Anmol Publications, Reprint 2004.
5. Harish Kumar, Industrial Chemistry, Sarup & Sons Reprint 2002.
6. J.E. Huheey, E.A. Keiter, R.L. Keiter, Inorganic Chemistry, Pearson Education Asia, Reprint 2001.
7. F.A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, John Wiley & Sons, 5th Edn., 1988.
8. B.E. Douglas, D.H. McDaniel and J.J. Alexander, Concepts and Models of Inorganic Chemistry, John Wiley & Sons, 2 Edn. 1983.
9. I. V. Kozhevnikov, Catalysis by Heteropoly Acids and Multicomponent Polyoxometalates in Liquid-Phase Reactions, *Chem. Rev.* **1998,** *98,* 171-198.
10. D. E. Katsoulis, A Survey of Applications of Polyoxometalates, *Chem. Rev.* **1998,** *98,* 359-387.

MCHIEC		
L (hrs)	Credits	Course
45	3	Elective

ELECTIVE PAPER III - INORGANIC

Nuclear Chemistry

Unit I Radioactivity And Its Measurement (09 hrs.)

Discovery – types of decay – decay kinetics – half-life period, mean life, parent-daughter decay – growth relationship – secular and transient equilibrium; Units of radioactivity; alpha, beta and gamma decay; Theory of decay, energies and properties – artificial radioactivity. Detectors: ionization chamber, electron pulse counter, scintillation detectors.

Unit II Nuclear Reactions (09 hrs.)

Bathe's notation – types of nuclear reactions: The compound nucleus theory – reaction cross section, transmutation reactions, elastic and inelastic scattering, spallation, fragmentation, stripping and pick-up; fission, fusion, photonuclear reactions and thermonuclear reactions.

Unit III Nuclear Reactors (09 hrs.)

The fission energy – reproduction factor; Classification of reactors based on moderators, coolants, phase of fuel and generation. Principle of thermal nuclear reactors: The four factor formula, reactor power, critical size of a thermal reactor, excess reactivity and control. Breeder reactor India's nuclear energy programmes – reprocessing of spent fuels.

Unit IV Radiation And Matter (09 hrs.)

Radiation chemistry – passage of radiation through matter – units for measuring radiation absorption – radiation dosimetry – radiolysis of water – free radicals in water radiolysis – chemical dosimetry: Radiolysis of Fricke Dosimeter solution – Radiation induced colour centres in crystals – Effects of radiation with matter. Radiolysis of inorganic gases, organic gases, organic compounds, solids and polymers – Annealing of radiation damage.

Unit V Applications Of Radioactivity (09 hrs.)

Application of radioisotopes: probing by isotopes, reactions involved in the preparation of radioisotopes. The Szilard-Chalmers' reaction – Radiochemical principles in the use of Tracers – Applications of radioisotopes as tracers – chemical investigations, analytical applications, agricultural and industrial applications – Neutron activation analysis – Carbon and rock dating .

References

1. S. Glasstone, Source book on atomic energy, East West press, 3rd Edn. 1967.
2. H.J. Arniker, Essentials of Nuclear Chemistry, New Age International, Reprint 2009.
3. M.G. Friedlander, J.M. Kennedy, E.S. Macian and J.M. Miller, Nuclear and Radiochemistry, 3rd Edn. John Wiley & Sons, 1981.
4. M.G. Arora and M. Singh, Nuclear Chemistry, Anmol Publications, 1994.
5. E.S.Gilreath, Fundamental concepts of Inorganic Chemistry, McGraw Hill 17th print 1982.

MCHPEA		
L (hrs)	Credits	Course
45	3	Elective

ELECTIVE PAPER I- PHYSICAL

Polymer Chemistry

Unit I **(09 hrs.)**

Concept of macromolecules – principle of duality – molecular design – nomenclature and classification – raw material sources of polymers – classification of polymers - synthetic schemes – Isolation and Purification of Polymers – Polymer fractionation – Molecular Weight determination, distribution curve – glass transition temperature - Petroleum and petrochemicals – oil refinery: a perceptive.

Unit II **(09 hrs.)**

Polymerization processes – free radical and addition polymerization; kinetics and mechanism, Chain transfer – molecular weight distribution and molecular weight control; Radical atom transfer and fragmentation – addition mechanism, Free radical living polymers, cationic and anionic polymerization- kinetics and mechanism; polymerization without termination; Living polymers, step growth polymerization – linear vs cyclic polymerization.

Unit III **(09 hrs.)**

Polymer Stereochemistry – configuration and conformation, tacticity – chiral polymers- stereoregularity in polymers – isotactic, syndiotactic and atactic polymers; polar and non-polar polymers; stereospecific polymerization and the utility of Ziegler-Natta catalyst; Copolymerization – bulk solution, melt, suspension, emulsion and dispersion techniques; synthesis of graft and block copolymers.

Unit IV **(09 hrs.)**

Polymer solutions – Flory-Huggins equation – Chain dimension – chain stiffness – End-to-end distance – conformation – random coil – Solvation ad Swelling – Flory-Reiner equation. Determination of degree of crosslinking and molecular weight between crosslinks.

Industrial polymers – Synthesis, Structure and applications of industrially important polymers.

Unit V **(09 hrs.)**

Conducting polymers – synthesis of conducting polymers - chemical structure and electronic behavior of polymers – doping of conducting polymers – p- & n- type doping – doping techniques; semiconducting properties of organic polymers containing

metal groups – semiconduction of biopolymers and its application to biochemical problems – superconductors.

References

1. F. W. Billmeyer, Textbook of polymer Science, 3rd Edn, Wiley, New York, 1991.
2. V. R. Gowariker, N. V. Viswanathan, J. Sreedhar, Polmer Science, Wiley-Eastern, New Delhi, 1988.
3. A. Tager, Physical Chemistry of Polymers, Mir Publishers, Moscow, 1978.
4. R. J. Young, Principles of Polymer Science, 3rd Edn., Chapman and Hall, New York, 1991.
5. P. J. Flory, Polymer Science, Cornell University Press, Ithacka, 1953.
6. J. E. Katon, Organic Semiconducting Polymers, Marcel Dekker, New York, 1968.
7. B. Bahadur, N. V. Sastry, Principles of Polymer Science, Narosa, New Delhi, 2002.

ELECTIVE PAPER II-PHYSICAL

Material Science and Nanoscience

MCHPEB		
L (hrs)	Credits	Course
45	3	Elective

Unit I Materials Chemistry and Synthesis (09 hrs.)

Solid state reaction: general principle, experimental methods, crystallization of solution, melts, glasses and gels; vapor phase transport method; synthesis of metastable phases by chimie dome; hydrothermal and high pressure methods.

Solid electrolytes: β-alumina and silver compounds and their applications.

Unit II Materials for specialized applications (09 hrs.)

Optical and photonic materials – overview –refractive index – optical dispersion and birefringence; passive optical materials –materials and devices for passive optical applications –lenses, prisms, filters –optical wave guide, responsive optical materials-liquid crystalline materials –Photochromic, electrochromic and non-linear optical materials –light emitting materials.

Unit III Nanomaterials – Introduction and types (09 hrs.)

Introduction to Nanoscience: Introduction- definition of nanoscience, nanochemistry- classification of the nanomaterials – Zero dimensional nanostructures-one dimensional nanostructures- nanowires and nanorods - two dimensional nanostructures-films, nanotubes and biopolymers-three dimensional nanostructures-fullerenes and dendrimers- quantum dots and their properties.

Unit VI Nanomaterials – Preparation and Properties (10 hrs.)

Synthesis of nanomaterials : Introduction – precipitative methods – hydrothermal and solvothermal methods - chemical methods - reduction methods – colloidal and micellar approach – sol-gel method – chemical vapor deposition method.

Properties of nanomaterials – physical properties – finite size effects – optical, magnetic and electronic properties – chemical properties – semiconductor nanoclusters – applications of nanomaterials.

Unit V Specialized Nanomaterials (08 hrs.)

Nanomaterials and their occurrence in nature, nanogold and glass materials – monolayer protected metal nanoparticles – Brust method of preparation, characterization and their applications – core-shell nanoparticles – metal-metal oxide, bimetallic, semiconductor and polymer-coated core-shell nanoparticles, electrical and optical properties and applications in biology, catalysis, sensing and chemical reactivity.

References

1. H. R. Allcock, Introduction to Materials Chemistry, John Wiley & Sons, Inc. Publication, 2008.
2. A. R. West, Solid State Chemistry and its applications, Wiley 2004.
3. M. T. Weller, Inorganic Materials Chemistry, Oxford Chemistry Primes, 1996.
4. W. Jones, Organic molecular solids, CRC Press, 1997.
5. T. Pradeep, Nano: The Essentials, Tata Mc Graw-Hill, 2007.

MCHPEC		
L (hrs)	Credits	Course
45	3	Elective

ELECTIVE PAPER III - PHYSICAL

Catalysis

Unit I **(09 hrs.)**

Catalysis phenomenon – mode of action of catalysts – classification of catalysts – Comparison of Homogeneous and Heterogeneous Catalysis. Homogeneous catalysis – general mechanisms; acid-base catalysis – catalytic activity, mechanisms and salt effects.

Enzyme catalysis – influence of substrate concentration, pH, temperature, and enzyme mechanisms. Kinetics of inhibition –chain reaction, enzyme catalyzed reactions.

Unit II **(10 hrs.)**

Catalysis in molecular-scale cavities – structure of crystalline solids – zeolites – families of zeolites; adsorption and diffusion in zeolites – catalysis by zeolites containing metal complexes and clusters; non-zeolite molecular sieves – clays and other layered materials.

Catalysis – catalysts for PTC – mechanism and benefits of PTC – PTC reactions – selected industrial processes with PTC.

Unit III **(08 hrs.)**

Micellar catalysis: effects of micelles on chemical reactions, characteristics of enzymatic reactions, micelle-catalyzed reactions, inhibition in micellar solutions; reverse micelles and microemulsions – catalysis in thermal and photochemical reactions.

Unit IV **(09 hrs.)**

Electrocatalysis – introduction to electrocatalysis and fuel cells – industrial application of catalysis – petroleum refining – distillation, cracking, reforming, hydrotreating, Alkylation and isomerization, ethylene-based processes – ethylene oxide and ethylene glycol, polyethylene, vinyl chloride and PVC; Propylene-based processes – acrylic acid and acrylonitrile, Ziegler-Natta chemistry; C$-based processes – butadiene, isobutylene.

Unit V **(09 hrs.)**

Surface catalysis – introduction – mechanism of surface reactions: Langmuir-Hinshelwood & -Rideal mechanisms; surface structures – single crystal surface of metals, high-surface area amorphous solids; adsorption; functionalized surfaces;

catalysis on functionalized surfaces: connection to molecular catalysis; catalysis on metal surfaces, metal oxide surfaces, mixed metal oxides, metal sulfides (minimum one example for each).

References:

1. B. C. Gates, Catalytic Chemistry, John Wiley & Sons, Inc., 1992.
2. J. C. Kuriacose, Catalysis, Macmillan India Ltd., New Delhi, 1991.
3. M. Gratzel, K. Kalyanasundaram, Eds., Kinetics and Catalysis in Microheterogeneous Systems, Marcel Dekker, New York, 1991.
4. K. Kalyanasundaram, Photochemistry in Microheterogeneous Systems, Academic Press, Orlando, 1987.
5. K. J. Laidler, Chemical Kinetics, 3rd Edition, Pearson Education Pte., Ltd., 2005.
6. P. H. Emmett, Catalysis, Vol. I and II, Reinhold Corp., New York, 1954.
7. J. M. Smith, Chemical Engineering Kinetics, McGraw Hill, 1971.
8. J. Hagen, Industrial Catalysis: A Practical Approach, 2nd Edition, Wiley-VCH, 2006.

PRACTICALS

ORGANIC PRACTICAL - III

MCHL41		
L (hrs)	Credits	Course
60	2	Practical

Advanced Organic Chemical Analysis

1. Distillation Methods:Fractional distillation, Azeotropic Distillation, Distillation under reduced pressure and Steam distillation.
2. **S**eparation of organic compounds: Paper chromatography, TLC and Column chromatography.
3. Characterization of organic compounds: UV, FT-IR, Gas chromatography (GC), and LCMS.

References

1. R.M. Silverstein, G.C. Bassler, T.C. Morril, Spectrometric Identification of Organic Compounds, John Wiley & Sons, New York, 1991.
2. W. Kemp, Organic Spectroscopy, Macmillan Press Ltd. 1996.
3. Jag Mohan, Organic Spectroscopy, Principles and Applications, Narosa publishing House, New Delhi, 2001.
4. P. R.Young, Practical Spectroscopy, The Rapid Interpretation of Spectral Data Brooks/Cole, California, 2000.
5. R. Davis, M. Frearson, Mass Spectrometry, John Wiley & Sons, New York, 1991.

INORGANIC PRACTICAL - III

MCHL42		
L (hrs)	Credits	Course
60	2	Practical

Advanced Inorganic Chemical Analysis

Preparation of Metal complexes/compounds and their characterization by UV VIS & IR spectral, chromatographic and other physico-chemical techniques. Some typical examples of complexes/compounds are as follows.

1. Tris(acetylacetonato)manganese(III)
2. Potassium trioxalatochromate(III)
3. Tris(thiourea)copper(I) sulphate
4. Cis & trans-potassium dioxalatodiaquochromate(III)
5. Tris(ethylenediamine)chromium(III) chloride
6. Nitro- and nitrito-pentamminecobalt(III) chloride
7. Tetramminecopper(II) sulphate
8. Hexamminecobalt(III) chloride
9. Hexathiourealead(II) nitrate

Some typical analyses are:

1. Determination of Δ_o of metal complexes by UV VIS spectroscopy
2. Confirmation of metal-ligand bond & complex formation by IR spectroscopy
3. Determination of conductivity of ionic type metal complexes
4. Determination of composition of metal complexes by UV VIS spectral Job's method
5. Identification of cis & trans isomers by chemical and spectral methods
6. Determination of magnetic susceptibility by Gouy method and confirmation of high & low spin states of complexes

References:

1. G. Pass & H. Sutcliffe, Practical Inorganic Chemistry, Science paperbacks, Chapman and Hall, London, 1974.
2. R. Gopalan & V. Ramalingam, Concise Coordination Chemistry, Vikas Publishing House Pvt. Ltd., NewDelhi 2001
3. R.S. Drago, Physical Methods in Chemistry, W.B. Saunders, 1997.
4. E.A. V. Ebsworth et al., Structural Methods in Inorganic Chemistry, ELBS 1987.

PHYSICAL CHEMISTRY PRACTICAL - III

MCHL43		
L (hrs)	Credits	Course
60	2	Practical

Advanced Physical method of Chemical Analysis

Part 1: Spectrophotometry

a. Mixture analysis - Determination of concentration of two components in a given mixture ($KMnO_4$& $K_2Cr_2O_7$).

b. Determination of metal ions (lead, calcium, magnesium) from water samples using calibration curve method.

Part 2: Electrochemical analysis

a. Determination of redox potentials of organic and inorganic molecules.

b. Amperometric titration of $Pb(NO_3)_2$ with $K_2Cr_2O_7$.

Part 3: Surface analysis (atleast one)

a. Surface area analysis and pore size measurement using BET surface analyzer from porous materials.

b. Analysis of crystal structure from single crystal/powder X-ray pattern.

Part 4: pHmetry

a. Determination of dissociation constants of tribasic acid (phosphoric acid).

b. Determination of some physical parameters of water samples (eg.: alkalinity).

References:

1. A. Findary, T. A. Kitchner, Practical physical chemistry. (Longmans, Green and Co.)
2. J. M. Wilson, K. J. Newcombe, A. R. Denko, R. M. W. Richett, Experiments in Physical Chemistry, (Pergamon Press).
3. D. P. Shoemaker, C. W. Garland, Experiments in Physical Chemistry, McGraw-Hill. New York, 1967.

MANONMANIAM SUNDARANAR UNIVERSITY, TIRUNELVELI-12

DEPARTMENT OF CHEMISTRY

L (hrs)	Credits	Course
60	3	MOOCS

Supportive Course (other department students)

Even Semester / Second Semester

Paper I –Chemistry and Environment (3 Credits)

Unit I Environment and Ecology (09 hrs.)

Introduction to environment – concept and scope, environmental segments. Ecosystem and environment. The natural cycles (H_2O, O_2, N_2) of environment. Environmental pollution and its classification.

Unit II Air Pollution (09 hrs.)

Atmosphere – composition, structure and evolution; green house effect and global warming; photochemical smog and acid rain. Ozone hole and El Nino phenomenon. Different types of air pollutants and sources; air quality standards.

Unit III Water Pollution (09 hrs.)

Different types of water pollutants and sources. Eutrophication; heavy metal ions (Hg, Pb and Cr) poisoning; fluoride and defluoridation. Water quality standards.

Unit IV Soil Pollution (09 hrs.)

Composition of soil; micro and macronutrients; wastes and pollutions in soil; disposal of municipal, medical and industrial wastes. Plants as indicators of soil pollution.

Unit V Environmental restoration (09 hrs.)

Environmental restoration; recycling and further use of waste. Conservation of forests and wild life. The state of global environment and earth summit.

References:

1. A.K. De, Environmental Chemistry, New Age publishers, New Delhi, 3, 4 & 5th Edn., 2003.
2. B.K. Sharma and H.Kaur, Environmental Chemistry, Goel Publishing House, Meerut, 3rd Edn., 1996.
3. G.S. Sodhi, Environmental Chemistry, Narosa Publishing House, New Delhi, 2000.

Supportive course

Odd Semester / Third Semester

Paper II – Chemistry and Industry (3 credits)

Unit I Petroleum Products **(09 hrs.)**

Petroleum – its occurrence, mining, composition and classification; distillation of crude petroleum; gasoline for motor and aeroplanes, diesel and kerosene, knocking and anti-knocking; octane and cetane number; pyrolysis of heavy oil and production of gasoline.

Unit II Plastics **(09 hrs.)**

Natural and Synthetic polymers, plastics – thermosetting and thermoplastic and their general methods of preparation; synthesis of important plastics and their applications – polythene, polypropylene, nylon, polyester, PVC and Bakelite.

Unit III Soaps and Detergents **(09 hrs.)**

Soap – hard & soft – manufacture; toilet, laundry, shaving and other types of soaps; cleaning action of soap.

Detergents – their different types and manufacture.

Unit IV Fertilizers **(09 hrs.)**

Fertilizers – different types and their requirement; manufacture of urea, ammonium phosphate, superphosphate and potassium sulphate and their utilization; complex fertilizers; micronutrients.

Unit V Cement **(09 hrs.)**

Portland and other types of cement; manufacture of Portland cement-wet and dry processes; settling of cement; cement industry in India.

References:

1. B.K. Sharma, Industrial Chemistry, Goel publication, Ist revised Edn., 1993.
2. M.G. Arora, M. Singh, Industrial Chemistry Vol. 1 & 2 Anmol publication, Ist Edn., 1994
3. B.N. Chakrabarthy, Industrial Chemistry, Oxford & IBH, 5th reprint 1991.