

**Syllabus
and
Course Structure
Choice Based Credit System**

for

M. Sc. Chemistry
To be implemented from
Academic session-2016-17



Department of Chemistry
Faculty of Science
JAMIA HAMDARD
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Hamdard Nagar, New Delhi-110062

M.Sc. PROGRAMME IN CHEMISTRY COURSES OF STUDY

I SEMESTER

Paper Code	Title of the Paper	Paper Category	Semester Exam	Internal Assessment	Total Marks	Hours per week		Course Credit
						L	P	
MFC -001	Foundation Course	Foundation	150	50	200	08	00	08
MCHCC -101	Physical Chemistry - I	Core	75	25	100	03	00	03
MCHCC -102	Organic Chemistry - I	Core	75	25	100	03	00	03
MCHCC-103	Inorganic Chemistry - I	Core	75	25	100	03	00	03
MCHCC-104	Lab. Course in Physical Chemistry- I	Core	75	25	100	00	06	03
MCHCC-105	Lab. Course in Inorganic Chemistry - I	Core	75	25	100	00	06	03
MCHCC-106	Lab. Course in Organic Chemistry-I	Core	75	25	100	00	06	03
Total: I Semester			600	200	800	17	18	26

II SEMESTER

Paper Code	Title of the Paper	Paper Category	Semester Exam	Internal Assessment	Total Marks	Hours per week		Course Credit
						L	P	
MCHCC -201	Physical Chemistry - II	Core	75	25	100	03	00	03
MCHCC -202	Organic Chemistry - II	Core	75	25	100	03	00	03
MCHCC -203	Inorganic Chemistry - II	Core	75	25	100	03	00	03
MCHCC -204	Analytical Chemistry	Core	75	25	100	03	00	03
MCHCC-205	Applications of Spectroscopy	Core	75	25	100	03	00	03
MCHCC-206	Lab. Course in Physical Chemistry- II	Core	75	25	100	00	06	03
MCHCC-207	Lab. Course in Inorganic Chemistry - II	Core	75	25	100	00	06	03
MCHCC-208	Lab. Course in Organic Chemistry-II	Core	75	25	100	00	06	03
Total: II Semester			600	200	800	15	18	24
Total: I Semester and II Semester			1200	400	1600			50

Specialization in Organic Chemistry

III SEMESTER

Paper Code	Title of the Paper	Paper Category	Semester Exam	Internal Assessment	Total Marks	Hours per week		Course Credit
						L	P	
MCHCCO - 301	Chemistry of Natural Products - I	Core	75	25	100	03	00	03
MCHCCO- 302	Organic Synthesis – I	Core	75	25	100	03	00	03
MCHCCO - 303	Photochemistry and Pericyclic reactions	Core	75	25	100	03	00	03
MCHDCE-304/305/306	Discipline Centric Elective – I	Discipline Specific Elective	75	25	100	03	00	03
MCHOE-307	Environmental chemistry	Generic elective	75	25	100	03	00	03
MCHCCO -308	Lab. Course	Core	150	50	200	00	20	10
Total: III Semester			525	175	700	15	20	25

IV SEMESTER

Paper Code	Title of the Paper	Paper Category	Semester Exam	Internal Assessment	Total Marks	Hours per week		Course Credit
						L	P	
MCHCCO - 401	Chemistry of Natural Products - II	Core	75	25	100	03	00	03
MCHCCO - 402	Organic Synthesis – II	Core	75	25	100	03	00	03
MCHCCO- 403	Heterocyclic Chemistry	Core	75	25	100	03	00	03
MCHDCE-404/405/406	Discipline Specific Elective - II	Discipline Specific Elective	75	25	100	03	00	03
MCHOE-407	Chemistry in Nanoscience	Generic elective	75	25	100	03	00	03
MCHDCE – 408	Project	Project	150	50	200	00	20	10
Total: IV Semester			525	175	700	15	20	25
Total: III & IV Semester			1050	350	1400			50
Grand Total: Sem I-IV					3000			100

Specialization in Industrial Applications

III SEMESTER

Paper Code	Title of the Paper	Paper Category	Semester Exam	Internal Assessment	Total Marks	Hours per week		Course Credit
						L	P	
MCHCCI - 309	Food Chemistry-I	Core	75	25	100	03	00	03
MCH CCI- 310	Polymer Chemistry-I	Core	75	25	100	03	00	03
MCHCCI - 311	Medicinal Chemistry-I	Core	75	25	100	03	00	03
MCHDCE-304/305/306	Discipline Specific Elective – I	Discipline Specific Elective	75	25	100	03	00	03
MCHOE-307	Environmental chemistry	Generic elective	75	25	100	03	00	03
MCHCCI -312	Lab. Course I	Core	150	50	200	00	20	10
Total: III Semester			525	175	700	15	20	25

IV SEMESTER

Paper Code	Title of the Paper	Paper Category	Semester Exam	Internal Assessment	Total Marks	Hours per week		Course Credit
						L	P	
MCHCC - 409	Food Chemistry – II	Core	75	25	100	03	00	03
MCHCCI – 410	Polymer Chemistry – II	Core	75	25	100	03	00	03
MCHCCI- 411	Medicinal Chemistry-II	Core	75	25	100	03	00	03
MCHDCE-404/405/406	Discipline Specific Elective - II	Discipline Specific Elective	75	25	100	03	00	03
MCHOE-407	Chemistry in Nanoscience	Generic elective	75	25	100	03	00	03
MCHCCI- 412	Lab.course-II	Core	75	25	100	03	14	07
MCHDCE – 413	Project	Project	75	25	100	00	-	03
Total: IV Semester			525	175	700	15	14	25
Total: III & IV Semester			1050	350	1400			50
Grand Total: Sem I-IV					3000			100

List of Discipline Specific Elective Papers:

Paper Code	Paper Title	Paper Code	Paper Title
MCHDCE-304	Medicinal Chemistry	MCHDCE-404	Polymer Chemistry
MCHDCE-305	Catalysis and Green Chemistry	MCHDCE-405	Bioorganic and Bioinorganic Chemistry
MCHDCE-306	Advanced methods of chemical analysis	MCHDCE-406	Molecular Modelling & Drug Design

- Student is required to opt for one Discipline specific elective course of 03 credits each in semester III and Semester IV apart from project work in semester IV.
- Student is required to opt for Open elective paper(s) of minimum 06 credits from any discipline/subject of his or her choice offered in any department of the university including his own department towards award of M.Sc. in Chemistry.
- A Discipline Centric elective paper will be taught in the department if at least 40 % students of the ongoing batch opt for it.
- An open elective course will be taught in the department if more than 5 students opt for it.
- In case of foundation course, M.Sc. Chemistry students are not required to take up foundation course for Chemistry.

I Semester

M.Sc. CHEMISTRY
PHYSICAL CHEMISTRY-I
MCHCC-101

50 Hours

Unit – I

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 determination of fugacity.

Non-ideal systems: Excess functions for non-ideal solutions, activity, activity coefficient, Debye-Hockel theory for activity coefficient of electrolytic solutions; determination of activity and activity coefficients.

Application of phase rule of three component systems; second order phase transitions

Unit – II

Electrochemistry of solutions: Debye-Huckel-Onsager treatment and its extension, ion solvent interactions. Debye-Huckel-Jerum mode. Thermodynamics of electrified interface equations. Derivation of electro-capillarity, Lippmann equations (surface excess), methods of determination. Structure of electrified interfaces. Guoy-Chapman, Stern, Graham-Devanathan-Mottwatts, Tobin, Bockris, Devanathan models. Over potentials, exchange current density, derivation of Butler-Volmer equation, Tafel plot. Semiconductor interfaces- theory of double layer at semiconductor, electrolyte solution interfaces.

Applications of electrochemistry in energy, e.g., Hydrogen cell, Li-battery, solar cell, fuel cells. Electrocatalysis-influence of various parameters, Hydrogen electrode.

Bioelectrochemistry, threshold membrane phenomena, Nernst-Planck equation, Hodgkin-Huxley equations, core conductor models, electrocardiography, electrodialysis. Polarography theory, Ilkovic equation; half wave potential and its significance.

Unit – III

Quantum mechanics: The Schrodinger equation and the postulates of quantum mechanics. Discussion of solutions of the Schrodinger equation to some model systems viz., particles in a box, the harmonic oscillator, the rigid rotor, the hydrogen atom, Hamiltonian Operator, Position Operator, Linear momentum and Angular momentum Operator, Commutation of operator, Commutation of angular momentum and position (Heisenberg principle), Eigen Value and Eigen Functions, Normalisation and orthogonality of Ψ . Determination of position and momentum of particle in one dimensional box from Ψ expression.

Unit – IV

Adsorption: Surface tension, capillary action, pressure difference across curved surface (Laplace equation), vapour pressure of droplets (Kelvin equation), Gibbs and Langmuir adsorption isotherms, estimation of surface area (BET equation), surface films on liquids (electro-kinetic phenomenon), catalytic activity of surfaces. Catalysis- Concept of traditional catalysts and nano catalysts and their application in industry.

Books recommended

1. Physical Chemistry, P.W.E. Atkins, ELBS
2. Introduction Quantum Chemistry, A.K. Chandra, Tata Mc Graw Hill.
3. Quantum Chemistry, I.N. Levine, Prentice Hall.
4. Coulson's valence, R. McWeeny, ELBS
5. Thermodynamics, J. Rajaram; J.C. Kuriacose, Educational Publishers.
6. Physical Chemistry of surfaces, A.W. Adamson, John Wiley and Sons.
7. Quantum Chemistry, E. Walter, Kinball publications

8. Statistical Physics (Part I) (Course of Theoretical Physics Vol. 5), L.D. London; E.M. Lifshitz, Pergamon press.
9. Modern Electrochemistry Vol I and Vol II, J.O.M. Bockris ; A.K.N. Reddy, Plenum publication
10. Electrochemistry by Bockris
11. Quantum Chemistry by McQuerry

M.Sc. CHEMISTRY
ORGANIC CHEMISTRY-I
MCHCC-102

50 Hours

Unit I

Nature of Bonding in Organic Molecules: Delocalized chemical bonding-conjugation, cross conjugation, resonance, hyperconjugation, bonding in fullerenes, tautomerism. Aromaticity in benzenoid and non-benzenoid compounds, alternant and non-alternant hydrocarbons, Huckel's rule, energy level of π -molecular orbitals, annulenes, anti-aromaticity, Ψ -aromaticity, homo-aromaticity, PMO approach. Bonds weaker than covalent- addition compounds, crown ether complexes and cryptands, inclusion compounds- cyclodextrins, catenanes and rotaxanes.

Unit II

Stereochemistry: Conformational analysis of cycloalkanes, decalins, effect of conformation on reactivity, conformation of sugars, steric strain due to unavoidable crowding. Elements of symmetry, chirality, molecules with more than one chiral center, threo and erythro isomers, methods of resolution, optical purity, enantiotopic and diastereotopic atoms, groups and faces, stereospecific and stereoselective synthesis. Asymmetric synthesis. Optical activity in the absence of chiral carbon (biphenyls, allenes and spiranes), chirality due to helical shape. Stereochemistry of the compounds containing nitrogen, sulphur and phosphorus.

Unit III

Reaction Mechanism: Structure and Reactivity: Types of mechanisms, types of reactions, thermodynamic and kinetic requirements, kinetic and thermodynamic control, 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, free radicals, carbenes and nitrenes. Effect of structure on reactivity- resonance and field effects, steric effect, quantitative treatment. The Hammett equation and linear free energy relationship, substituent and reaction constants. Taft equation.

Unit IV

Aliphatic and Aromatic Nucleophilic Substitution: The S_N2 , S_N1 , mixed S_N1 and S_N2 and SET mechanisms. The neighbouring group mechanism, neighbouring group participation by π and σ bonds, anchimeric assistance. Classical and nonclassical carbocations, phenonium ions, norbornyl system, common carbocation rearrangements. Application of NMR spectroscopy in the detection of carbocations. The S_N1 mechanism. Nucleophilic substitution at an allylic, aliphatic trigonal and a vinylic carbon. Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium, phase transfer catalysis and ultrasound, ambident nucleophile, regioselectivity. The S_NAr , S_N1 , benzyne and $S_{RN}1$ mechanisms. Reactivity – effect of substrate structure, leaving group and attacking nucleophile. The Von Richter, Sommelet-Hauser and Smiles rearrangements Hydrolysis of esters and amides, Ammonolysis of esters.

Books Recommended:

1. Advanced Organic Chemistry-Reactions, Mechanism and Structure, Jerry March, John Wiley.
2. Advanced Organic Chemistry, F.A. Carey and R.J. Sundberg, Plenum.
3. A Guide Book to Mechanism in Organic Chemistry, Peter Syks, Longman
4. Structure and Mechanism in Organic Chemistry, C.K. Ingold Cornell University Press
5. Organic Chemistry, R.T. Morrison and R.N. Boyd, Prentice-Hall.
6. Modern Organic Reactions, H.O. House, Benjamin.
7. Principles of Organic Synthesis, R.O.C. Norman and J.M. Coxon, Blackie Academic & Professional.
8. Reaction Mechanism in Organic Chemistry, S.M. Mukherji and S.P. Singh, Macmilan.
9. Stereochemistry of Organic Compounds, D. Nasipuri, New Age International.
10. Stereochemistry of Organic Compounds, P.S. Kalsi, New Age International.

M.Sc. CHEMISTRY
INORGANIC CHEMISTRY-I
MCHCC-103

UNIT-I

Chemical periodicity & Structure of molecules and stereochemical non-rigidity: Fundamental trends-First and second row anomalies-The diagonal relationship-The use or not of d orbitals by nonmetals- periodic anomalies of nonmetals and post transition elements-inert pair effect- - VSEPR rules-Structures of molecules containing lone pairs of electrons-Walsh diagrams-AH₂ molecules-Bent's rule -covalent radii- van der Waals radii- Experimental determination of molecular structure- atomic inversion- Berry pseudo-rotation-fluxional organometallic compounds-Effects of chemical forces-melting, boiling points and solubility.

UNIT-II

Concepts of acids and bases- Non-aqueous solvents- Main group elements: Bronsted & Lowry-Lewis & Flood-Lewis definitions-a generalized acid-base concept- measures of acid-base strength-Steric & solvation effects and acid base anomalies-Hard-Soft acid base concept- acid base strength and hardness and softness- symbiosis-theoretical basis- effect of electronegativity-Non-aqueous solvents-ammonia- sulphuric acid-protonic solvents-aprotic solvents-molten salts-hydrometallurgy- Main group elements- allotropy, synthesis, structure and bonding of their compounds- Boron cage compounds-higher boranes- classifications-Wades's rules-carboranes-metallacarboranes-structure predictions for heteroboranes.

UNIT-III

Transition elements and coordination compounds: valence bond theory-hybridization-inner orbital-outer orbital complexes-crystal field theory-octahedral-tetrahedral -tetragonal symmetries-crystal field stabilization energy-factors affecting CFSE-Molecular orbital theory of octahedral, tetrahedral and square planar complexes-p-bonding and molecular orbital theory-electronic spectra-term symbols and splitting of terms- correlation-Orgel and Tanabe-Sugano diagrams-calculations of Dq, B and b parameters- tetragonal distortions and Jahn-Teller theorem-LMCT and MLCT-spectra-magnetic properties of complexes-substitution reactions in square planar and octahedral metal complexes- trans effect-aquation and anation reactions-reaction rates influenced by acids and bases- redox reactions- inner sphere and outer sphere reaction mechanisms- excited state outer sphere electron transfer reactions.

UNIT-IV

Inner transition elements & Bioinorganic chemistry: The lanthanide and actinide elements- stable oxidation states- lanthanide-actinide contraction- the f-orbitals- absorption spectra- magnetic properties- coordination chemistry-comparison with transition metal complexes- Lanthanide chelates- transactinide elements- periodicity of transactinide elements- Bioinorganic chemistry: photosynthesis- chlorophyll- porphyrins- heme group-cytochromes- metalloenzymes, carboxy peptidase- carbonic anhydrase- hemoglobin- myoglobin and oxygen transport, dioxygen complexes-vitamin B₁₂ and coenzyme B₁₂-electron- transfer reactions; iron-sulphur proteins-rubredoxins and ferredoxins- blue copper proteins- hemocyanins and hemerythrins- nitrogenases- nitrogen cycle and *in vivo* nitrogen fixation, metal complexes in medicine- cis platin- essential and trace elements in biological systems.

Books Recommended:

1. Advanced Inorganic Chemistry, 6th ed. - F.A. Cotton, G. Wilkinson, Wiley 1999
2. Inorganic Chemistry, 4th ed. - J.E. Huheey, Harpis and Row
3. Inorganic Chemistry- Wulfsberg (Viva, 20020
4. Chemistry of the Elements 2nd ed. – N.N. Greenwood, A. Earnshaw, Pergaman
5. Inorganic Chemistry, 3rd ed. – D.F. Shriver, P.W. Atkins (Oxford, 1999)
6. Coordination Chemistry – D. Banerjee (Tata McGraw Hill, 1993)

M.Sc. CHEMISTRY
LAB COURSE IN PHYSICAL CHEMISTRY -I
MCHCC-104

40 hours

The experiments shall be covered from the following practical course:

pH-metry

1. Determination of strength and pK value of a weak acid by titration with an alkali.
2. Determination of degree of hydrolysis of aniline hydrochloride.

Refractometry

3. Determination of refractive index of some liquids and finding the composition of a binary liquid mixture by refractivity method.
4. Determination of molar refraction, molar polarization and electron polarisability of liquids.

Spectrophotometry

5. Establishing the validity of Beer-Lambert law.
6. Determination of composition of a binary mixture of $K_2Cr_2O_7$ and $KMnO_4$.

Viscometry

7. Investigation of variation of viscosity with conc. and determination of unknown concentration.
8. Determination of the radius of a molecule by viscosity measurement.

Chemical Kinetics

1. Study of kinetics of hydrolysis of an ester catalysed by dil. HCl.
2. Determination of order of reaction between $K_2S_2O_8$ and KI by Initial rates method.

Calorimetry

3. Determination of heat of neutralization of a strong acid with a strong base.
4. Determination of heat of neutralization of a weak acid with a strong base.

Books Recommended

1. Practical Physical Chemistry, Findley, Kitchener, Longman, 1977.
2. Advanced Practical Physical Chemistry, Yadav, Goel Pub, 1994.
3. Experiments in Physical Chemistry, 5th ed., Schoemaker et al., MGH, 1989.

I Semester

**M.Sc. CHEMISTRY
LAB COURSE IN INORGANIC CHEMISTRY -I
MCHCC-105**

40 hours

The experiments shall be covered from the following practical course:

Qualitative Analysis:

- a) Systematic qualitative analysis and identification of cations using group reagents including those of less common elements, Tl, Mo, W, Ti, Zr, Th, V, U, Li.
- b) Identification of anions including insoluble sulphates, oxides and halides.

Chromatography:

- c) Paper chromatographic separation of ions such as (i) Ag(I) & Pb(II); (ii) Cu(II), Pb(II), Bi(III) & Cd(II); (iii) Ni(II), Co(II) & Zn(II); (iv) Ba(II), Sr(II) & Ca(II); (v) F⁻, Cl⁻, Br⁻ & I⁻
- d) Column chromatographic (on ion exchange resin) separation and estimation of strength of (i) Zn(II) & Mg(II).

Books Recommended

1. Vogel's qualitative Inorganic Analysis; 6th edn; Svehla (Longman, 1994)
2. The physical Chemistry of Inorganic Qualitative analysis; Kuriacose, Rajaram (Tata MGH, 1972)
3. Vogel's Textbook of Quantitative chemical Analysis; 5th edn; Jeffery, Bassett; (ELBS, 1989)
4. Quantitative Analysis; 6th edn; Day, Underwood (Printice Hall, 1993).
5. Chromatographic Methods; 3rd ed; Stock & Rice (Chapman & Hall, 1980).
6. Analytical Chemistry; 5th ed; D. Christian (Wiley)

M.Sc. CHEMISTRY
LAB COURSE IN ORGANIC CHEMISTRY -I
MCHCC-106

40 hours

The experiments shall be covered from the following practical course:

1. Qualitative Analyses of mono and bifunctional compounds
 - a. Detection of Functional Groups
 - b. Group tests for compounds of natural origin
2. Determination of specific rotation and resolution of racemic mixtures
3. Quantitative estimation of the following:
Carbohydrates, amino acids, proteins, Carboxylic acids, Phenols/Aniline
4. Separation, Purification and Identification of Organic compounds from a two component mixture
Separation based on solubility in water.
Separation based on solubility in organic solvents.
Separation based on chemical properties: Solubility in Sodium Bicarbonate, Sodium Hydroxide and Hydrochloric acid
5. Analytical and preparative TLC
6. Small scale organic synthesis
 - i. Preparation of oximes (acetophenone oxime/ cyclohexanone oxime/vanillin oxime)
 - ii. Preparation of 2,4-dinitrophenylhydrazone
 - iii. Preparation of isoamyl acetate
 - iv. Preparation of substituted acetamide and benzamide from amines.
 - v. Alkylation, sulphonation, nitration and chlorination of aromatic compounds
 - vi. Preparation of p-bromoacetanilide from Aniline
 - vii. 2- and 4-nitrophenols (nitration and separation by steam distillation)
 - viii. Cyclohexanol from cyclohexanone (LAH reduction)
 - ix. Preparation of adipic acid from oxidation of cyclohexanol by chromic acid
 - x. Benzimidazole from benzyl
 - xi. Preparation of dibenzalacetone.
7. UV and IR of simple organic compounds for functional group identification

Books Recommended

1. Experiments and Techniques in Organic Chemistry, D. Pasto, C. Johnson and M. Miler, Prentice Hall
2. Macroscale and Microscale Organic Experiments, K.L. Williamson, D.C. Heath
3. Vogel's Textbook of Practical Organic Chemistry, A.R. Tatchell, John Wiley

4. Chemistry of Natural Products: A laboratory Handbook by N.R. Krishnaswamy, University Press, 2003
5. Comprehensive Practical Organic Chemistry, V.K. Ahluwalia, Renu Agarwal (University Press India Ltd.-2000)
6. Organic Laboratory techniques, Donald C Pavia, Gary M Lampman.
7. Experimental Organic Chemistry John C Gilgert, Stephen F Martin.(SCP)
8. Advanced Practical Organic Chemistry, Vol.II, Jagmohan (Himalaya Publishing House)

**M.Sc. CHEMISTRY
PHYSICAL CHEMISTRY-II
MCHCC-201**

50 Hours

Unit I

Chemical Dynamics I: Methods of determining rate laws, collision theory of reaction rates, steric factor, activated complex theory, Arrhenius equation and the activated complex theory; ionic reactions, kinetic salt effects, steady state kinetics, kinetic and thermodynamic control of reactions, treatment of unimolecular reactions.

Dynamic chain (hydrogen-bromine reaction, pyrolysis of acetaldehyde, decomposition of ethane), photochemical (hydrogen-bromine and hydrogen-chlorine reactions) and oscillatory reactions (Belousov-Zhabotinsky reaction)

Unit II

Chemical Dynamics II: Homogeneous catalysis, kinetics of enzyme reactions, general features of fast reactions, study of fast reactions by flow method, relaxation method, flash photolysis and the nuclear magnetic resonance method. Dynamics of molecular motions, probing the transition state, dynamics of barrierless chemical reactions in solution, dynamics of unimolecular reactions (Lindemann-Hinshelwood and Rice-Ramsperger-Kassel-Marcus [RRKM] theories of unimolecular reactions).

Unit – III

Concept of distribution, thermodynamic probability and most probable distribution: Ensemble averaging, postulates of ensemble averaging. Canonical, grand canonical and microcanonical ensembles, corresponding distribution laws using Lagrange's method of undetermined multipliers). Partition functions: translational, rotational, vibrational and electronic partition functions, calculation of thermodynamic properties in terms of partition functions. Fermi-Dirac statistics, distribution law and applications to metal. Bose-Einstein statistics – distribution law and application to helium.

Unit – IV

Micelles: Surface active agents, classification of surface active agents, micellization, hydrophobic interaction, critical micellar concentration (CMC), factors affecting the CMC of surfactants, counter ion binding to micelles, thermodynamics of micellization phase separation and mass action models, solubilization, micro emulsion, reverse micelles.

Books recommended

1. Physical Chemistry, P.W. Atkins, ELBS
2. Chemical Kinetics, K.J. Laidler, McGraw Hill
3. Kinetics and Mechanism of Chemical Transformations, J. Rajaraman ; J. Kuriacose, McMillan publications
4. Micelles, Theoretical and Applied Aspects, V. Moroi, Plenum Publications.
5. Statistical Mechanics by D. Nash

M.Sc. CHEMISTRY
ORGANIC CHEMISTRY – II
MCHCC-202

50 Hours

Unit I

Aliphatic Electrophilic Substitution: Bimolecular mechanisms- S_N2 and S_N1 . The S_N1 mechanism, electrophilic substitution accompanied by double bond shifts. Effect of substrates, leaving group and the solvent polarity on the reactivity.

Aromatic Electrophilic Substitution: 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, Vilsmeier reaction, Gattermann-Koch reaction.

Unit II:

Free Radical Reactions: Types of free radical reactions, free radical substitution mechanism, mechanism at an aromatic substrate, neighbouring group assistance. Reactivity for aliphatic and aromatic substrates at a bridgehead. Reactivity in the attacking radicals. The effect of solvents on reactivity. Allylic halogenation (NBS), oxidation of aldehydes to carboxylic acids, auto-oxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salts. Sandmeyer reaction. Free radical rearrangement. Hunsdiecker reaction.

Unit III

Addition to Carbon-Carbon Multiple Bonds: Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, regio- and chemoselectivity, orientation and reactivity, addition of cyclopropane ring, hydrogenation of double and triple bonds, hydrogenation of aromatic rings, hydroboration, Michael reaction, Sharpless asymmetric epoxidation. Addition to Carbon-Hetero Multiple Bonds: mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds acids, esters and nitriles, addition of Grignard reagents, organozinc and organolithium reagents to carbonyl and unsaturated carbonyl compounds, Wittig reaction, mechanism of condensation reactions involving enolates – Aldol, Knoevenagel, Claisen, Mannich, Benzoin, Perkin and Stobbe reactions.

Unit IV

Elimination Reactions: The $E2$, $E1$ and $E1cB$ mechanisms and their spectrum. Orientation of the double bond. Reactivity – effects of substrate structures, attacking base, the leaving group and the medium. Mechanism and orientation in pyrolytic elimination.

Books Recommended:

1. Advanced Organic Chemistry-Reactions, Mechanism and Structure, Jerry March, John Wiley.
2. Advanced Organic Chemistry, F.A. Carey and R.J. Sundberg, Plenum.
3. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman
4. Structure and Mechanism in Organic Chemistry, C.K. Ingold Cornell University Press
5. Organic Chemistry, R.T. Morrison and R.N. Boyd, Prentice-Hall.
6. Modern Organic Reactions, H.O. House, Benjamin.
7. Principles of Organic Synthesis, R.O.C. Norman and J.M. Coxon, Blackie Academic & Professional.
8. Reaction Mechanism in Organic Chemistry, S.M. Mukherji and S.P. Singh, Macmillan.
9. Stereochemistry of Organic Compounds, D. Nasipuri, New Age International.
10. Stereochemistry of Organic Compounds, P. S. Kalsi, New Age International.

M.Sc. CHEMISTRY
INORGANIC CHEMISTRY - II
MCHCC-203

50 Hours

UNIT-I

Organometallic compounds: 18 electron rule and counting electrons in complexes- metal carbonyl complexes- poly nuclear carbonyl complexes- carbonylate ions- carbonyl hydride complexes - isolobal fragments- Structural predictions for organometallic clusters- nitrosyl complexes- dinitrogen complexes- metal alkyls- carbenes- carbenes and carbide-alkyl complexes-non aromatic alkene and alkyne complexes- metallocenes- structures of cyclopentadienyl compounds- covalent versus ionic bonding- arene complexes- cycloheptatriene and tropylium complexes- substitution reactions in carbonyl complexes- ligand cone angles- oxidative addition and reductive elimination- insertion and elimination reaction- alkene hydrogenation and Wilkinson catalyst- Tolmann catalytic loops- synthesis gas- hydroformylation- Wacker process-synthetic gasoline- Ziegler-Natta catalysis.

UNIT-II

Inorganic rings, cages, polymers and metal clusters: synthesis, structure and bonding of S-N compounds- B-N compounds- P-N compounds- theories of bonding in phosphazenes-phosphazene polymers and applications-other heterocyclic ring systems- heterocatenation- silicates- intercalation compounds- isopoly acids- hetero poly acids- synthesis, structure and bonding in metal clusters- di-, tri-, tetra-, and hexa-nuclear clusters- poly atomic Zintl anions and cations- Chevrel phases- infinite metal chains.

UNIT-III

Inorganic spectroscopy: Characterisation of inorganic compounds by IR, symmetry and shapes of AB_2 , AB_3 , AB_4 , AB_5 , AB_6 mode of bonding of ambidentate ligands, ethylene diamine and diketonato complexes- application of resonance Raman spectroscopy for the study of active site of metalloproteins- EPR spectroscopy- hyperfine coupling-g-tensors- application to transition metal complexes having one unpaired electron-including biological systems and inorganic free radicals- NMR spectroscopy of paramagnetic substances- contact and pseudo contact shifts-some applications of ^{31}P , ^{195}Pt and ^{119}Sn NMR spectroscopy- Mössbauer, basic principles-spectral parameters and spectrum display- application to the study of bonding and structures of Fe^{2+} , Fe^{3+} including those of intermediate spin.

UNIT-IV

Chemical applications of group theory & Solid state: symmetry elements- symmetry operations- mirror plane-center of symmetry -rotational axis- identity- improper rotation- point groups and molecular symmetry- irreducible representations and character tables- uses of point group symmetry-infrared and Raman spectroscopy- selection rules- Solid state: crystallography- crystal systems and Bravais lattices- Bragg's law and applications; the ionic bond- structures of crystal lattices- lattice energy- the Born-Haber cycle- factors affecting the radii of ions-efficiency of packing and crystal lattices- radius ratio- covalent character in ionic solids- imperfections in crystals-conductivity in ionic solids- types of solids- band structure of solids- high temperature super conductors.

Books Recommended:

1. Advanced Inorganic Chemistry, 6th ed- F.A. Cotton, G. Wilkinson, Wiley 1999
2. Inorganic Chemistry, 4th ed. - J.E. Huheey, E.A. Keiter, Harpiss and Row
3. Chemistry of the Elements 2nd ed. – N.N. Greenwood, A. Earnshaw, Pergamon
4. Mechanisms of Inorganic Reactions – D. Katakis, G. Gordon (Wiley, 1987)
5. Reaction Mechanism of Inorganic and Organometallic systems, 2nd ed. – R.B. Jordan (Oxford, 1998).
6. Mechanisms of Inorganic Reactions, 2nd ed. – F. Basolo, R.G. Pearson (Wiley, 1967).
7. Inorganic Chemistry – K.F. Purcell, I.C. Kutz (Saunders, 1977).
8. Electronic Spectra of Transition Metal Complexes – D. Sutton (McGraw-Hill, 1968)
9. Elements of Magnetochemistry – R.L. Dutta, A. Syamal (Affiliated East – West, 1993).
10. Inorganic Electronic Spectroscopy, A.B.P. Lever, Elsevier
11. Magnetochemistry, R.L. Carlin, Springer Verlag
12. Comprehensive Coordination Chemistry Eds., G. Wilkinson, R.D. Gillies and J.A. McCleverty, Pergamon

M.Sc. CHEMISTRY
ANALYTICAL CHEMISTRY
MCHCC-204

50 Hours

Unit I

Adsorption/Partition Chromatography: Kinds of adsorption interactions, adsorption characteristics, chromatographic mechanism, classification of chromatography.

TLC- Principle, phases-silica, alumina, plate loading-analytical vs. preparative, visualization, limits of detection and quantitation, factors affecting separation

Column Chromatography. Principle, types and techniques of column chromatography, techniques of elution. Theoretical aspects - theoretical plates, K-values, solute mobilities. Operating parameters.

Unit II

Gas-liquid chromatography: Instrumentation, carrier gas, columns, solid supports, liquid phases, coating of support, sample preparation and introduction, retention time, Applications of GC.

High Performance Liquid Chromatography: Instrumentation- mobile phase reservoirs, pumping system, sample injection system, columns, detectors, operating parameters, retention times vs. volumes. Reverse phase HPLC, chiral HPLC, semi-preparative and preparative HPLC, Applications of HPLC.

Unit III

Size Exclusion chromatography: Theory. Supports- Hydrophilic gels, soft gels, hard gels, organo and lipophilic gels.. Experimental design- choice of column, support and eluent, optimization of flow rate and loading. Experimental methods- column preparation, sample application. Applications- desalting, molecular weight and polydispersity determination, determination of equilibrium constant,

Ion exchange chromatography: Resins- strong acid and base, weak acid and base. working parameters, chromatographic procedures - displacement chromatography, elution chromatography, gradient elution, column load, size and flow rate, column packing, solvent choice, liquid ion exchangers applications of ion exchangers.

Unit IV

Nuclear Radiation methods: Nuclear reactions and radiations, interaction of nuclear radiation with matter, radioactive decay measurements, ionization chamber, proportional counter, Geiger-Muller counter, scintillation counter, semi-conductor detectors,

Thermal and Calorimetric methods of Analysis: Basics, methodology and applications of Thermogravimetric analysis, Differential thermal analysis and Derivative thermogravimetry. Interpretation of TGA and DTA curves of important compounds e.g., calcium oxalate monohydrate, magnesium oxalate monohydrate. Analysis of silver-copper alloy and dolomite

Books recommended

1. Fundamentals of Analytical chemistry, D. A. Skoog; D. M. West; F. J. Holler, Harcourt college publications.
2. Principles and practice of analytical chemistry, F. W. Fildes; D. Kealey, Blackwell publication.

3. Analytical chemistry, G.D. Christian, Wiley and sons publication.
4. Handbook of instrumental techniques for analytical chemistry, F. A Settle, Prentice Hall Publication.
5. Analytical chemistry- Instrumental Techniques (Vol. II); M. Singh, Dominant publishers.
6. Basic concepts of analytical chemistry, S. M. Kopper, New Age International Publishers.
7. Analytical chemistry, D. Kealey, P.J.Haines, Viva books Pvt. Ltd.

M.Sc. CHEMISTRY
APPLICATIONS OF SPECTROSCOPY TO STRUCTURAL ANALYSIS
MCHCC-205

50 Hours

Unit I**Ultraviolet, Visible and Luminescence Spectroscopy:**

Introduction, wave-like propagation of light, absorption of electromagnetic radiation by organic molecules, allowed and forbidden transitions, absorption laws and molar absorptivity, electronic transitions, spectrophotometer and spectrum recording, effect of solvents on electronic transitions, formation and designation of absorption bands, conjugated systems and transition energies, unsaturated carbonyl compounds, dienes and conjugated polyenes, Woodward – Fieser rules. UV spectra of aromatic, heterocyclic compounds and steric effect in biphenyls. General applications of ultraviolet spectroscopy.

Introduction to fluorescence and Phosphorescence. Fluorescence lifetime and quantum yields, fluorescence anisotropy, instrumentation for fluorescence spectroscopy, effects of solvents on fluorescence emission spectra, mechanism and dynamics of solvent relaxation, quenching of fluorescence, applications of fluorescence spectroscopy. Principle of phosphorescence spectroscopy and its applications.

Unit II

Infrared Spectroscopy: Introduction, absorption in the infrared region, theory of infrared spectroscopy, molecular vibrations, calculation of vibrational frequencies, factors affecting vibrational frequencies, characteristic absorptions in common classes of compounds, fingerprint region, characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ether, phenols and amines. Detailed study of vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters, acids, anhydrides, lactones, lactams and conjugated carbonyl compounds), applications of infrared spectroscopy, interpretation of infrared spectra of organic compounds. IR of gaseous, solids and polymeric materials. Instrumentation – CWIR and FTIR. Basics of Raman Spectroscopy

Unit III

NMR Spectroscopy: Introduction, theory of NMR spectroscopy, vector model, Bloch equation, multiplicity, instrumentation, chemical shift, H-1 NMR spectroscopy- equivalent and nonequivalent protons, vicinal coupling and stereo structure, proton exchange reactions, nuclear overhauser effect (NOE), shift reagents, principle of FT – NMR. C-13 NMR spectroscopy, multiplicity- ¹H decoupling, noise decoupling, off- resonance decoupling, DEPT ¹³C spectra, introduction to ¹⁵N, ³¹P and ¹⁹F NMR. Interpretation of NMR spectra of some representative compounds. Introduction of 2D NMR spectroscopy, Coherence transfer, Coherence selection, Pulse sequences - COSY, Hetero-COSY, NOESY, Interpretation of 2D NMR spectra of some representative compounds.

Unit IV

Mass Spectrometry: Introduction, basic theory, instrumentation, important useful terms in mass spectrometry, various modes of ionization (EI, CI, FD, FAB, ESI and MALDI) and their applications, fragmentation patterns of various functional group molecular ion peak, metastable peak, McLafferty rearrangements, nitrogen rule, GC-MS, LC-MS and their applications. Introduction to MS-MS.

Books recommended

1. Introduction to spectroscopy, Pavia; Lampman , Kriz, Books/cole.
2. Spectroscopic methods in organic chemistry, H. Williams; I. fleminig, Tata Mc Grawhills
3. Organic spectroscopy, W. Kemp, Palgrave publications.
4. Fundamentals of Analytical chemistry, D. A. Skoog; D. M. West; F. J. Holler, Harcourt college publications.
5. Principles and practice of analytical chemistry, F. W. Fifield; D. Kealey, Blackwell publication.
6. Analytical chemistry, G.D. Christian, Wiley and Sons publication.
7. Spectrometric identification of organic compounds, R. M. Silverstein, John Wiley and Sons publication.
8. Basic concepts of analytical chemistry, S. M. Kopper, New Age International Publishers.
9. Analytical chemistry, D. Kealey; P.J.Haines, Viva books Pvt. Ltd
10. Analytical Chemistry – Instrumental techniques, Vol. I, M. Singh, Dominent publication

M.Sc. CHEMISTRY
LAB COURSE IN PHYSICAL CHEMISTRY – II
MCHCC-206

40 hours

The experiments shall be covered from the following practical course:

Conductometry

1. Determination of the composition of a mixture of HCl and CH₃COOH by titration with standard NaOH.
2. Determination of degree of dissociation of weak acid.

Phase Equilibria

3. Determination of the transition temperature of a solid.
4. Study of the phenol/water and carbon disulphide/methanol system.

Potentiometry

5. Determination of strength of an acid by titration with an alkali using quinhydrone electrode
6. Titration of Fe (II) vs K₂Cr₂O₇ and determination of standard redox potential of Fe²⁺/Fe³⁺.

Polarimetry

5. Determination of the specific rotation of an optically active compound and determination of unknown concentration from the calibration curve.
6. Determination of the rate constant of inversion of cane sugar catalysed by HCl.

Books Recommended

1. Practical Physical Chemistry, Findley, Kitchener, Longman, 1977.
2. Advanced Practical Physical Chemistry, Yadav, Goel Pub, 1994.
3. Experiments in Physical Chemistry, 5th ed., Schoemaker et al., MGH, 1989.

**M.Sc. CHEMISTRY
LAB COURSE IN INORGANIC CHEMISTRY – II
MCHCC-207**

40 hours

The experiments shall be covered from the following practical course:

Preparation of coordination compounds of transition metals and their characterization by IR and electronic spectra:

- (i) $\text{VO}(\text{acac})_2$
- (ii) $\text{TiO}(\text{C}_9\text{H}_8\text{NO})_2 \cdot 2\text{H}_2\text{O}$
- (iii) $\text{Cis-K}[\text{Cr}(\text{C}_2\text{O}_4)_2(\text{H}_2\text{O})_2]$
- (iv) $\text{Na}[\text{Cr}(\text{NH}_3)_2(\text{SCN})_4]$
- (v) $\text{Mn}(\text{acac})_3$
- (vi) $\text{K}_3[\text{Fe}(\text{C}_2\text{O}_4)_3]$
- (vii) Prussian Blue, Turnbull's Blue
- (viii) $[\text{Co}(\text{NH}_3)_6][\text{Co}(\text{NO}_2)_6]$
- (ix) $\text{Cis-}[\text{Co}(\text{trien})(\text{NO}_3)_2]\text{Cl} \cdot \text{H}_2\text{O}$
- (x) $\text{Hg}[\text{Co}(\text{SCN})_4]$
- (xi) $\text{Co}(\text{Py})_2\text{Cl}_2$
- (xii) $[\text{Ni}(\text{NH}_3)_6]\text{Cl}_2$
- (xiii) $\text{Ni}(\text{dmg})_2$
- (xiv) $[\text{Cu}(\text{NH}_3)_4]\text{SO}_4 \cdot \text{H}_2\text{O}$

Quantitative Analysis

- (a) Estimation of cations in dication using gravimetric and volumetric (complexometric or redox or iodometric argentometric titrations) methods like (i) Cu-Ni, (ii) Ni-Zn, (iii) Cu-Fe, (iv) Ag-Zn, (v) Fe-Ni, (vi) Cu-Mg, (vii) Ca-Mg, (viii) Zn-Mg.

Books Recommended

1. Vogel's qualitative Inorganic Analysis; 6th edn; Svehla (Longman, 1994)
2. The physical Chemistry of Inorganic Qualitative analysis; Kuriacose, Rajaram (Tata MGH, 1972)
3. Vogel's Textbook of Quantitative chemical Analysis; 5th edn; Jeffery, Bassett; (ELBS, 1989)
4. Quantitative Analysis; 6th edn; Day, Underwood (Printice Hall, 1993).
5. Chromatographic Methods; 3rd ed; Stock & Rice (Chapman & Hall, 1980).
6. Analytical Chemistry; 5th ed; D. Christian (Wiley)

M.Sc. CHEMISTRY
LAB COURSE IN ORGANIC CHEMISTRY – II
MCHCC-208

40 hours

The experiments shall be covered from the following practical course:

A: Preparation of the following

1. 2-Phenyl indole (Fischer indole synthesis),
2. 7-Hydroxy -3-methyl flavone (Baker-Venkatraman reaction),
3. Benzyl alcohol and benzoic acid from benzaldehyde (Cannizzaro reaction)
4. 4-Chlorotoluene from p-toluidine (Sandmeyer reaction)
5. Benzilic acid from benzoin (Benzilic acid rearrangement)
6. Benzopinacol from benzophenone (Photochemical reaction),
7. 7-Hydroxy-4-methyl coumarin (Pechmann Reaction)
8. 4-Methyl benzophenone (Friedel Craft reaction)
9. Benzanilide from benzophenone (Beckmann rearrangement)
10. Vanillyl alcohol from vanillin (NaBH₄ reduction)
11. Stilbene from benzyl chloride (Wittig reaction)
12. Ethyl cinnamate from benzaldehyde (Wittig reaction)
13. Triphenyl or diphenyl methyl carbinol (Grignard reaction)
14. Benzotriazole
15. 1-Phenyl-3-methyl pyrazol-5-one
16. Glucose pentaacetate
17. 2,4-diethoxycarbonyl-3,4-dimethyl pyrrole from ethyl acetoacetate
18. Quinoline from aniline Skraup synthesis)

B: Isolation of the following natural products.

19. nicotine dipicrate from tobacco.
20. caffeine from tea
21. eugenol from clove oil.
22. R (+) Limonene and Hesperidin from orange peel.
23. lycopene from tomatoes.
24. piperine from black pepper.
25. β -carotene from carrots.
26. lawsone from *Lawsonia alba*
27. atropine from datura seeds

Books Recommended

1. Experiments and Techniques in Organic Chemistry, D. Pasto, C. Johnson and M. Miler, Prentice Hall
2. Macroscale and Microscale Organic Experiments, K.L. Williamson, D.C. Heath
3. Vogel's Textbook of Practical Organic Chemistry, A.R. Tatchell, John Wiley
4. Chemistry of Natural Products: A laboratory Handbook by N.R. Krishnaswamy, University Press, 2003

5. Comprehensive Practical Organic Chemistry, V.K. Ahluwalia, Renu Agarwal (University Press India Ltd.-2000)
6. Organic Laboratory techniques, Donald C Pavia, Gary M Lampman.
7. Experimental Organic Chemistry John C Gilgert, Stephen F Martin.(SCP)
8. Advanced Practical Organic Chemistry, Vol.II, Jagmohan (Himalaya Publishing House)

Specialization in Organic Chemistry

Core Papers: III Semester

M.Sc. CHEMISTRY CHEMISTRY OF NATURAL PRODUCTS -I MCHCCO-301

50 Hours

Unit I

Terpenoids and Carotenoids: Classification, nomenclature, occurrence, isolation, general methods of structure determination, isoprene rule.

Structure determination and synthesis of the following representative molecules: Menthol, α -Terpeneol, Santonin, Abietic acid and β -amyrin. Biosynthesis of Terpenoids

Unit II

Alkaloids: Definition, nomenclature and physiological action, occurrence, isolation, general methods of structure elucidation, classification based on nitrogen heterocyclic ring and role of alkaloids in plants.

Structure, synthesis and biosynthesis of the following representative molecules: Nicotine, Atropine, Quinine and Morphine.

Unit III

Steroids: Occurrence, nomenclature, basic skeleton, Diel's hydrocarbon and stereochemistry. Isolation, structure determination and synthesis of cholesterol, bile acids, testosterone, progesterone. Biosynthesis of steroids.

Unit IV

Plant Pigments: Occurrence, nomenclature and general methods of structure determination. Isolation and synthesis of Apigenin, Quercetin, Myrcetin, Diadzein, Cyanidin and Hirsutidin.

Biosynthesis of flavonoids: Acetate pathway and Shikimic acid pathway.

Books recommended

1. Natural products: Chemistry and Biological Significance, J. Mann; R. S. Davidson; J. B. Hobbs; D. V. Banthrope ; J. B. Harborne, Longman publication.
2. Organic Chemistry, Vol 2, I. L. Finar, ELBS.
3. Stereoselective Synthesis: A practical Approach, M. Nogradi, VCH
4. Rodd's Chemistry of Carbin compounds, Ed. S. Coffey, Elsevier
5. Chemistry, Biological and Pharmacological Properties of Medicinal Plants from the Americas, Ed. K. Hostettmann; M. P. Gupta; A. Marston, Harwood Academic Publishers.
6. Introduction to Flavonoids, B.A.Bohm,Harwood Academic Publishers
7. Chemistry of natural products, S.V. Bhat; B. A. Nagasampagi; M. Sivakumar.
8. Biosynthesis of Natural products, P.Manitto, Ellis Horwood publishers.
9. Natural products from plants, P.B. Kaufman; L. J. Creke; S. Warber; J. A. Dupe; H. L. Briemann, CRC publication.
10. New Trends in Natural Product Chemistry, Att-ur-Rahman and M.I.Choudhary, Harwood Academic Publishers
11. Insecticides of Natural Origin, Sukh Dev, Harwood Academic Publishers

M.Sc. CHEMISTRY
ORGANIC SYNTHESIS – I
MCHCCO-302

50 Hours

Unit – I

Organometallic Reagents: Principle, preparations, properties and applications of the following in the organic synthesis with mechanistic details.

Group I and II Metal Organic compounds: Li, Mg, Hg, Cd & Zn compounds.

Transition metals: Cu, Pd, Ni, Fe, Co and Rh compounds.

Metallocenes and non-benzenoid aromatics- general considerations, synthesis and reactions of some representative compounds

Unit – II

Oxidation: Introduction, different oxidative processes. Hydrocarbons- alkenes, aromatic rings, saturated C-H groups (activated and unactivated). alcohols, diols, aldehydes, ketones, and ketals, amines, hydrazines, sulphides. Oxidizing agents- Jones reagent, LTA, HIO₄, Peracids, KMnO₄, OsO₄, SeO₂, Ruthenium tetroxide, Iodobenzenediacetate and Thallium (III) nitrate.

Unit – III

Reduction: Introduction, different reductive processes, Hydrocarbons- alkenes, alkynes and aromatic rings. Carbonyl compounds: Aldehydes, ketones, acids and their derivatives. Epoxides, nitro, nitroso, azo and oxime groups, Hydrogenolysis, Reducing agents – H₂/metal, Wilkinson catalyst, Lindlars catalyst, LAH, NaBH₄, Birch, Clemmenson Wolf Kishner and B₂H₆ reductions.

Unit – IV

Rearrangements: General mechanistic considerations- nature of migration, migratory aptitude, memory effects.

A detailed study of the following rearrangements:

Pinacol-pinacolone, Wagner Meerwein, Demjanov, Benzil-Benzilic acid, Favorskii, Arndt-Eistert Synthesis, Neber, Beckmann, Hofman, Curtius, Schmidt, Baeyer Villiger, Shapiro reaction.

Books recommended

1. Modern Synthetic reactions, W.A.Benjamin, H.O. House
2. Some Modern Methods of Organic Synthesis, W. Caruthers Cambridge University Press
3. Advanced Organic Chemistry, Reaction Mechanism and structure, Jerry March, John Wiley
4. Principles of Organic Synthesis, R. O.C Norman and J.M. Coxon, Blackie Academic and Professional
5. Advanced Organic Chemistry Part B, F.A. Carey, R. J. Sundberg, Plenum Press
6. Rodd's Chemistry of Carbon compounds, Ed. S. Coffey, Elsevier.

M.Sc. CHEMISTRY
PHOTOCHEMISTRY AND PERICYCLIC REACTIONS
MCHCCO-303

50 Hours

Unit I

Photochemical reactions: Interaction of electromagnetic radiation with matter, types of excitation, fate of excited molecule, quantum yield, transfer of excitation energy, actinometry.

Determination of reaction mechanism: Classification, rate constants and life times of reactive energy states-determination of rate constants of reactions. Effect of light intensity on the rate of photochemical reactions. Types of photochemical reactions- photo-dissociation, gas-phase photolysis

Unit II

Photochemistry of alkenes: Intramolecular reactions of the olefinic bond- geometrical isomerism, cyclisation reactions, rearrangement of 1,4- and 1,5-dienes.

Photochemistry of Carbonyl compounds: Intramolecular reactions of carbonyl compounds-saturated, cyclic and acyclic, β,γ -unsaturated and α, β -unsaturated compounds, Cyclohexadienones. Intermolecular cycloaddition reactions-dimerisations and oxetane formation

Unit III

Photochemistry of aromatic compounds: Isomerisations, additions and substitutions

Miscellaneous photochemical reactions: Photo-Fries reaction, Singlet molecular oxygen reactions, photochemical formation of smog. Photodegradation of polymers, Photochemistry of vision

Unit IV:

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. Cycloadditions-antarafacial and suprafacial additions, $4n$, $4n+2$ systems, $2+2$ addition of ketenes, 1,3 dipolar cycloadditions and cheletropic reactions.

Sigmatropic rearrangements-Suprafacial and antarafacial shifts of H, sigmatropic shifts involving carbon moieties, 3,3- and 5, 5- sigmatropic rearrangements, Claisen, Cope and aza-Cope rearrangements, Fuxional tautomerism, Ene reaction

Books recommended

1. Fundamentals of Photochemistry, K.K. Rohtagi-Mukherji, Wiley-Eastern.
2. Essentials of Molecular Photochemistry, A. Gilbert and J. Baggott, Blackwell Scientific Publication.
3. Molecular Photochemistry, N.J. Turro, W.A. Benjamin.
4. Introductory Photochemistry, A. Cox and T. Camp, McGraw-Hill.
5. Photochemistry, R.P. Kundall and A. Gilbert, Thomson Nelson.
6. Organic Photochemistry, J. Coxon and B. Halton, Cambridge University Press.
7. Pericyclic Reactions, S.M. Mukherji, Macmillan, India.

M.Sc. CHEMISTRY
LAB COURSE-III
MCHCCO-308

100 hours

The experiments shall be covered from the following practical course:

1. Benzaldehyde → Benzalacetophenone → Epoxide
2. 4-Nitro toluene → 4-Nitro benzoic acid → 4-Amino benzoic acid
3. Resorcinol → 4-methyl-7-hydroxy coumarin → 4-Methyl-7-acetoxy coumarin
4. Cyclohexanone → Phenyl hydrazone → 1,2,3,4-Tetrahydrocarbazole
5. Hydroquinone → Hydroquinone diacetate → 1,2,4-Triacetoxy benzene
6. Acetanilide → p-Acetamidobenzene sulphonyl chloride → P. Acetamidobenzene sulphonamide
7. p-Amino phenol → p-Acetyl amino phenol → p-Ethoxy acetanilide
8. Hippuric acid → Azalactone → 4-Benzylidene 2-phenyl oxazol-5-one
9. p-Cresol → p-Cresyl benzoate → 2-Hydroxy-5-methyl benzophenone
10. Phthalimide → N-Benzylphthalimide → Benzylamine
11. o-Nitroaniline → o-Phenylene diamine → Benzimidazole
12. Phthalic acid → Phthalimide → Anthranilic acid → o-Chlorobenzoic acid
13. Benzyl cyanide → p-Nitrobenzyl cyanide → p-Nitro phenyl acetic acid
14. Hydroquinone → Hydroquinone diacetate → 2,5-Dihydroxy acetophenone
15. Cyclohexanone → Enamine → 2-Acetyl cyclohexanone
16. α -Pinene → Disiamyl borane → Pinanol
17. Base catalyzed aldol condensation using LiOH.H₂O as a Catalyst.
18. Bromination of trans-stilbene using sodium bromide and sodium bromate
19. [4+2] cycloaddition reaction in aqueous medium at room temperature
20. Benzil Benzilic acid rearrangement under solvent free condition
21. Thiamine hydrochloride catalyzed synthesis of benzoin from benzaldehyde
22. Clay catalyzed solid state synthesis of 7-hydroxy-4-methylcoumarin
23. Ecofriendly nitration of phenols and its derivatives using Calcium nitrate
24. Bromination of acetanilide using ceric ammonium nitrate in aqueous medium
25. Green approach for preparation of benzopinacolone from bezopinacol using iodine catalyst
26. Preparation of 1, 1-bis-2-naphthol under grinding at room temperature.
27. Solvent free aldol condensation between 3,4-dimethoxybenzaldehyde and 1-indanone 13. Solvent free quantitative solid phase synthesis of azomethines from substituted anilines and substituted benzaldehydes.
28. Sucrose to ethyl alcohol (Baker's yeast)
29. Asymmetric reduction of EAA by using Baker's yeast
30. Alkylation of diethyl malonate with an alkyl chloride using microwaves.
31. Alkylation of diethyl malonate or ethyl acetoacetate with an alkyl halides using phase transfer catalyst.

Books recommended

1. Practical Physical Chemistry, Findley, Kitchener, Longman, 1977.
2. Advanced Practical Physical Chemistry, Yadav, Goel Pub, 1994.
3. Experiments in Physical Chemistry, 5th ed., Schoemaker et al., MGH, 1989.
4. Vogel's qualitative Inorganic Analysis; 6th edn; Svehla (Longman, 1994
5. The physical Chemistry of Inorganic Qualitative analysis; Kuriacose, Rajaram (Tata MGH, 1972)
6. Vogel's Textbook of Quantitative chemical Analysis; 5th edn; Jeffery, Bassett; (ELBS, 1989)
7. Quantitative Analysis; 6th edn; Day, Underwood (Printice Hall, 1993).
8. Chromatographic Methods; 3rd ed; Stock & Rice (Chapman & Hall, 1980).
2. Analytical Chemistry; 5th ed; D. Christian (Wiley)
3. Comprehensive Practical Organic Chemistry, V.K. Ahluwalia, Renu Agarwal (University Press India Ltd.-2000)
4. Organic Laboratory techniques, Donald C Pavia, Gary M Lampman.
5. Experimental Organic Chemistry John C Gilgert, Stephen F Martin.(SCP)
6. Monograph on Green Chemistry Laboratory Experiments by Green Chemistry Task Force Committee, DST

Core Papers-IV Semester

M.Sc. CHEMISTRY CHEMISTRY OF NATURAL PRODUCTS -II MCHCCO-401

50 Hours

Unit I

Prostaglandins: Occurrence, nomenclature, classification, biogenesis and physiological effects. Synthesis of PGE₂ and PGF₂α

Simple phenolic compounds: Structure and properties of naphthoquinones, anthraquinones, anthranols, anthrones and dianthrones. Coumarins - Classification, simple coumarins and their derivatives, isolation and identification. Tannins – Introduction, classification, hydrolysable tannins, condensed tannins, biological activities of tannins

Unit II

Biopolymers: Classification, structure and properties of amino acids, primary structure of peptides – N-terminal amino acid determination, carboxyl terminal amino acid determination, partial hydrolysis of peptides, cyclic peptides, biologically active peptides, isoelectric points of proteins. Classification and properties of proteins, colour reaction of proteins, sequencing of proteins, conformation and structure of proteins- primary, secondary, tertiary and quaternary structure, coagulation and denaturation of proteins

Unit III

Fatty acids: Fatty acids and its reactions, biological importance of fatty acids and lipids, identification and extraction of lipids, even chain and odd chain fatty acids, saturated and unsaturated fats, ketone bodies, fatty acid metabolism, Biosynthesis of fatty acids and triglycerides, Complex Lipids - Glycerophospholipids: Structure and function of (Phosphatic acid, cardiolipin, Phosphatidyl serine, Phosphatidyl ethanolamine, Phosphatidyl Glycerol, Phosphatidylcholine, Phosphatidyl inositol, plasmalogens), Glycosphingolipids: Structure and function of (Sphingosine, ceramides & sphingomyelins, cerebroside, globosides, gangliosides, sulfatides), biological membranes, properties and function of lipid bilayers.

Unit IV

Carbohydrates: Introduction, Types of naturally occurring sugars: Deoxy-sugars, dihydrosugars, amino sugars, branched chain sugars. Classification, nomenclature. Structures of triose, tetrose, pentose, and hexoses. Determination of ring size of aldohexose and aldopentose, Chain lengthening and chain shortening of aldoses. Reactions at the anomeric centre, reactions at the non-anomeric centre. Sugar analysis by enzymatic methods. Structure and properties of polysaccharides – cellulose, starch, pectins and mucopolysaccharides- hyaluronic acid and chondroitin. Separation of carbohydrates.

Books recommended

1. Natural products: Chemistry and Biological Significance, J. Mann; R. S. Davidson; J. B. Hobbs, D. V. Banthorpe ; J. B. Harborne, Longman publication.

2. Organic Chemistry, Vol 2, I. L. Finar, ELBS.
3. Introduction to Flavonoids, B.A. Bohm, Harwood Academic Publishers.
4. New Trends in Natural Product Chemistry, Atta-Ur-Rahman; M. I. Choudhary, Harwood Academic Publishers.
5. Bioactive Natural Products, S.J. Cutler; H.J. Cutler, CRC press.
6. Chemistry of natural products, S.V. Bhat; B.A.Nagasampagi; M. Sivakumar, Narosa publications
7. Biosynthesis of Natural products, P. Manitto, Ellis Horwood publishers
8. Natural products from plants, P. B. Kaufman; L. J. Creke; S.Warber; J. A. Dupe, H. L. Brielmann, CRC publication
9. Organic chemistry of natural products, Vol. I, II, G. Chatwal, Himalya Publishing house.
10. Phytochemicals as bioactive agents, W. R. Bidlack; S. T. Omaye; M.S. Meskin; C. K.W. Topharm, Technomic publishers.
11. Drugs of Natural origin: A text book of Pharmacognosy, Gunnar Simuelsson, Swedish pharmaceutical press, Apotekarsocieteten.

M.Sc. CHEMISTRY
ORGANIC SYNTHESIS – II
MCHCCO-402

50 Hours

Unit – I

Disconnection Approach: An introduction to synthons and synthetic equivalents, disconnection approach, functional group inter-conversions, the importance of the order of events in organic synthesis, one group C-X and two C-X disconnections, chemoselectivity, reversal of polarity, cyclization reactions, amine synthesis.

Unit – II

One Group C-C Disconnections: Alcohols and carbonyl compounds, regioselectivity, alkene synthesis, Stereoselective synthesis of tri and tetra substituted olefins, use of acetylenes and aliphatic nitro compounds in organic synthesis

Two group C-C Disconnections: Diels Alder reaction, 1,3-difunctionalized compounds, α,β -unsaturated carbonyl compounds, control in carbonyl condensations, 1,5-difunctionalised compounds, Michael addition and Robinson annulation.

Unit – III:

Modern Synthetic Methods: Baylis-Hillman reaction, Kulinkovich reaction, Ritter reaction, Sakurai reaction, Tishchenko reaction and Ugi reaction. Brook rearrangement; Prins reaction, Bignelli synthesis

Construction of Ring Systems: Different approaches towards the synthesis of three, four, five and six-membered rings; photochemical approaches for the synthesis of four membered rings, oxetanes and cyclobutanes. Pauson-Khand reaction, Bergman cyclization; aromatic heterocycles in organic synthesis.

Protecting groups: Principle of protection of alcohol, amine, carbonyl and carboxyl groups.

Unit – IV

Synthesis of some complex molecules: Camphor, Longifoline, Cortisone, Reserpine, Vitamin D, Juvabione, Aphidicolin and Fredericamycin A

Books recommended

1. Designing Organic Synthesis, S. Warren, Wiley
2. Organic Synthesis – Concept, Methods and Starting Materials, J.Fuhrhop and G. Penzillin, Verlage VCH
3. Modern Synthetic reactions, W.A.Benjamin, H.O. House
4. Some Modern Methods of Organic Synthesis, W. Caruthers Cambridge University Press
5. Advanced Organic Chemistry, Reaction Mechanism and structure, Jerry March, John Wiley
6. Principles of Organic Synthesis, R. O.C Norman and J.M. Coxon, Blackie Academic and Professional
7. Advanced Organic Chemistry Part B, F.A. Carey, R. J. Sundberg, Plenum Press

M.Sc. CHEMISTRY
HETEROCYCLIC CHEMISTRY
MCHCCO-403

50 Hours

Unit – I

Nomenclature of Heterocycles : Replacement and systematic nomenclature (Hantzsch-Widman system) for monocyclic, fused and bridged heterocycles.

Aromatic Heterocycles : General chemical behaviour of aromatic heterocycles, classification (structural type), criteria of aromaticity (bond lengths, ring current and chemical shifts in ^1H NMR-spectra, empirical resonance energy, delocalization energy and dewar resonance energy, diamagnetic susceptibility exaltations).

Heteroaromatic reactivity and tautomerism in aromatic heterocycles.

Non-aromatic Heterocycles: Strain – bond angle and torsional strains and their consequences in small ring heterocycles. Conformation of six-membered heterocycles with reference to molecular geometry, barrier to ring inversion, pyramidal inversion and 1,3-diaxial interaction. Stereo-electronic effects- anomeric and related effects. Attractive interactions- hydrogen bonding and intermolecular nucleophilic- electrophilic interactions.

Unit – II

Small ring heterocycles: Three-membered and four-membered heterocycles- synthesis and reactions of aziridines, oxiranes, thiiranes, azetidines, oxetanes and thietanes.

Benzo-fused five- membered heterocycles: Synthesis and reactions including medicinal applications of benzopyrroles, benzofurans and benzothiophenes.

Unit – III

Six- membered heterocycles: With one heteroatom; Synthesis and reactions of pyryllium salts and pyrones and their comparison with pyridinium & thiopyrylium salts and pyridones. Synthesis and reactions of quinolininium and benzopyrylium salts, coumarins and chromones.

With two or more heteroatoms: Synthesis and reactions of diazines, triazines, tetrazines and thiazines.

Unit – IV

Seven and large- membered heterocycles: Synthesis and reactions of azepines, oxepines, thiepinines, diazepines thiazepines, azocines, diazocines, dioxocines and dithiocines.

Heterocyclic Systems Containing P, As, Sb and B: Heterocyclic rings containing phosphorus: introduction, nomenclature, synthesis and characteristics of 5- and 6-membered ring systems-phosphorinanes, phosphorines, phospholanes and phospholels.

Heterocyclic rings containing As and Sb: introduction, synthesis and characteristics of 5-and 6-membered ring systems. Heterocyclic rings containing B: introduction, synthesis, reactivity and spectral characteristics of 3-, 5- and 6-membered ring systems.

Books recommended

1. Heterocyclic Chemistry Vol. 1-3, R.R. Gupta, M. Kumar and V. Gupta, Springer Verlag.
2. The Chemistry of Heterocycles, T. Eicher and S. Hauptmann, Thieme.
3. Heterocyclic Chemistry, J.A. Joule, K. Mills and G.F. Smith, Chapman and Hall.
4. Heterocyclic Chemistry, T.L. Gilchrist, Longman Scientific Technical.
5. Contemporary Heterocyclic Chemistry, G.R. Newkome and W.W. Paudler, Wiley-Interscience.
6. An Introduction to the Heterocyclic Compounds, R.M. Acheson, John Wiley.
7. Comprehensive Heterocyclic Chemistry, A.R. Katritzky and C.W. Rees, eds. Pergamon Press.

**M.Sc. CHEMISTRY
PROJECT
MCHDCE-408**

Marks 200

The project shall comprise of the following three components viz Part A of 100, Part B of 50 and Part C of 50 marks each given as under.

Part A:

Each student will undertake a project work in the Department of Chemistry under the supervision of a faculty member who will assign a topic of current/general interest under the overall supervision of Head of Department. The student shall consult literature/internet and collect the relevant material. After the completion of the experiment(s), each student has to submit a project report by the deadline fixed for the same purpose.

Part B:

Each student will make a presentation of the work carried out on the assigned topic followed by viva voce on the date and time fixed for the purpose.

Part C:

Each student will be continuously evaluated for his performance in execution of his or her project work during the entire semester by the supervisor assigned by the department for him to supervise the project work

Specialization in Industrial Applications

Core Papers: III Semester

M.Sc. CHEMISTRY
FOOD CHEMISTRY- I
MCHCCI - 309

50 Hours

Unit I

Food additives I: Introduction, aroma substances-Impact Compounds of Natural Aromas, Threshold Value, Aroma Value, Off-Flavors, Food Taints, Aroma Analysis. Individual Aroma Compounds: Nonenzymatic Reactions, Enzymatic Reactions. Flavour enhancers: Monosodium Glutamate (MSG), 5_-Nucleotides, Maltol. Sugar substitutes: sweeteners, sweet taste-structural requirements, structure–activity relationships in sweet compounds. Saccharin, Cyclamate, Curculin and Miraculin, Gymnema silvestre Extract, Stevioside, Phyllodulcin, Glycyrrhizin, Dihydrochalcones, Aspartame, Speraspartame, Neotame. Food colours, Antioxidants-Inhibition of lipid peroxidation, antioxidant activity, antioxidants in food, natural antioxidants, synthetic antioxidants, synergists, prooxidative effect. Acids and bases used in food industries.

Unit II

Food additives II: Antimicrobial agents: Benzoic Acid, PHB-Esters, Sorbic Acid , Propionic Acid, Acetic Acid, SO₂ and Sulfite, Diethyl (Dimethyl) Pyrocarbonate, Ethylene Oxide, Propylene Oxide, Nitrite, Nitrate Antibiotics, Diphenyl, o-Phenylphenol, Thiabendazole, 2-(4-Thiazolyl) benzimidazole. Emulsifiers: emulsions, emulsifier action, structure and activity, HLB-Value, synthetic emulsifiers-Mono-, diacylglycerides and derivatives, sugar esters, sorbitan fatty acid esters, polyglycerol – polyricinoleate (PGPR), stearyl-2-lactylate. Humectants- polyols 1,2-propanediol, glycerol, mannitol, sorbitol. Thickening agents, gel builders- agar, alginates, carrageenans, gum arabic, gum tragacanth, starch, cellulose- alkyl cellulose, hydroxyalkyl cellulose, Carboxymethyl cellulose, Anticaking agents, Bleaching agents, Propellants, Modified atmospheric packaging, protective gases

Unit III

Food Microbiology: Microorganisms important in food microbiology; common foodborne bacteria, common genera of foodborne molds, common genera of foodborne yeasts, intrinsic and extrinsic parameters of foods that affect microbial growth, low-temperature food Preservation and characteristics of psychrotrophic microorganisms, high-temperature food preservation and characteristics of thermophilic microorganisms, preservation of foods by drying, indicators of food safety and quality, principles of quality control.

Unit IV

Food Toxicants: Toxic trace elements in food- Arsenic, Mercury, Lead, Cadmium; Veterinary medicines and feed additives - Antibiotics, Anthelmintics, Coccidiostats, Analysis; Polychlorinated biphenyls; Harmful Substances from Thermal Processes-Polycyclic Aromatic Hydrocarbons (PAHs), Furan, Acrylamide; Nitrate, Nitrite, Nitrosamines; Polychlorinated Dibenzodioxins (PCDD) and Dibenzofurans (PCDF); Food-borne illness – bacterial and fungal, Toxic compounds of microbial origin, mycotoxins.

Books recommended

1. Food Chemistry, Belitz ; Gosch, Springer – Verlag Bertin Heiderberg publication.
2. Principles of Human Nutrition, M. Eastwood, Chapman and Hall.
3. Food – The Chemistry of its Components, T.P. Coultate, Royal Soc. Chemistry.
4. Food additives, B. A. Larry; D. P. Michael, Food Science and Technology series (35), Morcel Dekker, Inc.
5. Introduction to food science, R. Parker, Delmar Learning publication.
6. Nutrition Science and application, Smolin L.A, Saunders College Publishing.
7. Human Nutrition and dietetics, J.S. Barrow; W.P.T James; Churchill, Livingstone publication.

M.Sc. CHEMISTRY
POLYMER CHEMISTRY-I
MCHCCI - 310

50 Hours

Unit I

Structure, classification and nomenclature of polymers: Physical properties of the polymers- Amorphous and crystalline arrangements- Amorphous state, Elasticity, Crystallinity, thermal transitions, effect of chemical structure on physical properties, solubility of polymers, molecular weight and molecular weight distribution, Steric arrangement

Unit II

Chain growth polymerization: Free radical polymerization process, kinetics, initiators, efficiency of initiators, chain growth, steric, polar and resonance effects in the propagation reaction, termination of polymeric reactions, chain transfer, control of molecular weight, inhibitors and retarders, Effect of reaction medium and temperature on chain polymerization, ceiling temperature, Autoacceleration

Ionic chain growth polymerization: Cationic polymerization- Kinetics, Initiators, propagation, and termination reactions. Anionic polymerization- Kinetics, Initiators, propagation, and termination reactions. Coordinated anionic polymerization, Heterogenous and homogenous Ziegler Natta catalysts

Unit III

Step growth polymerization: Mechanism, kinetics and statistics of linear step growth polymerization, Carother's equation, Co-polymerisation- mechanisms, kinetics, Copolymer equation, monomer reactivity ratio, graft polymerization and block copolymerization. Ring opening polymerization, kinetics, cationic, anionic and hydrolytic polymerization of lactams.

Unit IV

Characterization of polymers: molecular weight and molecular distribution: molecular weight determination by osmometry, light scattering, viscometry and gel permeation chromatography, end group analysis, TGA, DSC and DMA with suitable examples.

Books recommended

1. Principles of polymer chemistry, A Ravve, Kluwer Academic publications
2. Textbook of Polymer science, F. W. Billmeyer, John Wiley and Sons publication.
3. Polymer Science and technology, J. R. Fried, Prentice – Hall publication.
4. Principles of polymer systems, F. Rodriguez; C. Cohen; C.K. Ober; L.A. Archer, Taylor & Francis publication.
5. Introduction to polymers, R.J. Young; P.A. Lovell, Netron Thornes publications
6. Polymer chemistry – an introduction, M. D. Stevens, Oxford University press.

M.Sc. CHEMISTRY
MEDICINAL CHEMISTRY-I
MCHCCI - 311

50 Hours

Unit – I

Drug Design: Biological targets and concept of lock and key, agonists and antagonists, Natural products as guiding principles for drug discovery, with classic examples like quinine, Oil of winter green etc. SAR, Modified natural products as improved drugs with examples like etoposide, vincristine, (anti cancer) and new generation penicillin, concept of pharmacophore, Drug design inspired by natural products and biochemical pathways. Example of sulphanilamide/PABA. Wholly synthetic drugs history and development with examples like salvarsan, cisplatin, ibuprofen.

The commercial synthetic procedures, classification, mechanism of action, uses and structure activity relationship for selected drugs as included under units II, III and IV shall be covered.

Unit – II

(a) Antibiotics

Penicillin, Cephalosporins, Tetracyclines, Macrolides, Streptomycin, Chloramphenicol and Quinolones.

(b) Sulpha drugs

Sulphanilamide, Sulphathiazole, Sulphadiazine and Sulphaacetamide

Unit – III

(a) Antimalarials

Chloroquine phosphate, Primaquine and Mefloquine

(b) Antifungal Agents

Ketoconazole, Griseofulvin

(c) Anthelmintics

Albendazole, Mebendazole

Unit – IV

(a) Anti- tubercular

Isoniazid, Rifampicin, Pyrazinamide, and Ethambutol

(b) Anti-neoplastics

Melphalan, Chlorambucil, Cisplatin

(c) Anti-amoebics

Emetine, Metronidazole and Tinidazole

Books recommended

1. Medicinal chemistry by Ashtosh kar kar, New age international limited publishers, Daryaganj
2. Wilson and Gisvold's Textbook of organic medicinal and pharmaceutical chemistry, Edited by Robert F. Doerge.
3. Burgers Medicinal Chemistry, M.E. Wolff, John Wiley and Sons
4. Principles of Medicinal Chemistry by W.O. Foye. Varghese publishing house Mumbai
5. The pharmacological basis of therapeutics, L.S. Goodman, A. Gilman
6. The organic Chemistry of drug synthesis, D. Lednicer. L.A. Mitscher
7. Medicinal Chemistry by D. Sriram, P. Yogeeswari Published by Dorling Kindersely (India) Pvt. Ltd. Patpargang, New Delhi
8. Introduction to Medicinal Chemistry, A. Gringuage, Wiley-VCH
9. An Introduction to Drug Design, S.S. Pandeya and J.R. Dimmock, New Age International.
10. Goodman and Gilman's Pharmacological Basis of Therapeutics, McGraw-Hill.
11. Strategies for Organic Drug Synthesis and Design, D. Lednicer, John Wiley.

M.Sc. CHEMISTRY

Lab. Course

MCHCCI - 312

100 hours

The experiments shall be covered from the following practical course:

Preparation of sulphanilamide
Preparation of sulphaguanidine
Preparation of paracetamol
Preparation of barbituric acid and its sodium salt.
Preparation of Antipyrine
Preparation of Tolbutamide
Estimation of aspirin present in a given sample/drug.
Estimation of ascorbic acid present in a given sample/drug.
To assay of amoxycillin present in an injection.
To assay a drug containing paracetamol, ibuprofen and chlorzoxazone.
To assay a drug containing paracetamol and diclofenac sodium.
To assay a drug containing diazepam and diphenhydramine hydrochloride
To assay a drug containing aspirin and caffeine citrate.
Determination of calcium and protein content in food.
Determination of sugar content in jams.
Determination of fat content of cheese.
Estimation of salt content in butter.
Determination of alcohol in beverages by GC.
Identification of milk products by HPLC.
Analysis of preservatives in food products by HPLC.
Analysis of sweeteners in food products by HPLC.

Books recommended

1. Analytical chemistry of foods by Ceirwyn S. James, Aspen Publication, 1994
2. Food Chemistry Laboratory, Connie M Weaver, James Reuben Daniel, CRC Press, 2003
3. Practical pharmaceutical Chemistry by A.H.Beckett, Cbs, 2005
4. Quantitative analysis of drugs in pharmaceutical formulations, by P.D.Sethi, Unique Publishers, 1985

Core Papers: IV Semester

M.Sc. CHEMISTRY FOOD CHEMISTRY- II MCHCCI-409

50 Hours

Unit I

Milk and Dairy products: Physico-chemical properties of milk, composition of milk- Proteins, casein fractions, micelle formation, gel formation, whey proteins, carbohydrates, lipids, organic acids, minerals, vitamins, enzymes, plasmin, lactoperoxidase, Processing of milk- purification, creaming, heat treatment, homogenization, types of milk.

Milk products: Fermented Milk Products - Sour milk, yogurt; Cream; Butter- Cream separation and treatment, churning, packaging, products derived from butter; ice creams; condensed milk, dehydrated milk products; cheese- curd formation, ripening, processed cheese.

Other products: casein, caseinates and coprecipitates, lactose, whey products- whey powder, partially desugared whey protein concentrates, hydrolyzed whey syrups

Unit II

Food Products I: Cereals and cereal products: general anatomy, chemical composition, Wheat- individual constituents, milling. Wheat Flour- chemical assays, physical assays, baking tests. Corn, Rice, Rye, Oats, Barley- storage, milling and milling products.

Vegetables and their products: Composition- nitrogen compounds, carbohydrates, lipids, organic acids, phenolic compounds, aroma substances; storage; vegetable products-dehydrated vegetables, canned vegetables, frozen vegetables, pickled vegetables, vegetable Juices, vegetable pastes, vegetable powders.

Sugars and sugar alcohols: Nutritional/physiological properties, sucrose, production of beet sugar, production of cane sugar, other sources for sucrose production, packaging and storage, types of sugar, sugars produced from sucrose, Sugar alcohols-isomaltol, sorbitol, xylitol, mannitol.

Unit III

Food Products II Fruits and their products: Composition- nitrogen compounds, carbohydrates, lipids, organic acids, phenolic compounds, aroma substances, chemical changes during ripening of fruit, ripening as influenced by chemical agents, storage of fruits, fruit products- dried, canned, deep frozen, marmalades, jams and jellies, fruit juices, analysis

Eggs- Structure, physical properties and composition- Albumen- proteins, lipids, carbohydrates, minerals, vitamins, egg yolk- proteins, lipids, vitamins, storage of eggs, egg products, technically important properties.

Meat- Structure of muscle tissue, muscle tissue composition and function, color of meat, curing, reddening, postmortem changes in muscle, aging of meat, water holding capacity of meat, kinds of meat, meat analysis.

Unit IV

Food Products III: Honey- Production and types, processing, physical properties, composition, storage, utilization, artificial honey.

Coffee- Harvesting and processing, storing and packaging, composition, coffee products- instant coffee, decaffeinated coffee.

Tea- Harvesting and processing, storing and packaging, types, composition.

Cocoa - Harvesting and processing, composition, production of cocoa liquor, production of cocoa powder, chocolate production, storage

Alcoholic beverages- Raw materials, processing, composition, types of beer and wine. Spirits- production, Liquor from wine, fruit, cereals and sugarcane

Salt- Composition, production, salt substitutes

Vinegar- Composition, microbiological production, chemical synthesis,

Books recommended

1. Food Chemistry, Belitz ; Gosch, Springer – Verlag Bertin Heiderberg.
2. Food – The Chemistry of its Components, T.P. Coultate, Royal Soc. Chemistry.
3. Introduction to food science, R. Parker, Delmar Learning.
4. Food Safety and Toxicity, J.de vries, CRC press.
5. Food Analysis – Theory & Practice, S.N. Mahindru, Metropolitan Book Co. Ltd.
6. Fundamentals of cheese science, P. F. Fox; T. P. Guinee, Aspen Publications
7. Food Technology processing and laboratory control, F. Aylward, Agrobios Publications.

M.Sc. CHEMISTRY
POLYMER CHEMISTRY – II
MCHCCI-410

50 Hours

Unit I

Industrial polymers I: Polyolefins: polyethylene, polypropylene; polystyrene, polyvinyl chloride, polyvinylacetate, polyvinylalcohol, acrylic polymers-PMMA, polyacrylonitrile, polyacrylamide, fluoropolymers-PTFE, polyamides- nylons.

Unit II

Industrial polymers II: Polyesters: alkyds, polyethylene terephthalate, polycarbonates, polydienes- natural rubber, polyisoprenes, rubbers derived from butadiene, cellulose and related polymers- regenerated cellulose, cellulose nitrate, cellulose acetate, cellulose ethers, phenol-formaldehyde polymers, aminopolymers- urea formaldehyde resin, polyurethanes, epoxies-bisphenol A- epichlorohydrin epoxies

Unit III

Polymer processing: classification of polymer processing, extrusion and extruders, calendaring, film blowing, injection moulding, blow moulding, vacuum forming, rotational, transfer and compression moulding, fibre spinning, polymer additives.

Unit IV

Chemical reactions of polymers: Addition reactions- halogenation, hydrogenation, electrophillic addition of aldehydes; polar additions- michael condensation, hydroboration, diel's alder condensation; Rearrangement reactions- isomerization reactions; Substitution reactions: Friedel-craft alkylation reactions, nitration and sulfonation reactions of polymers with aromatic rings, cross linking reactions of polymers, formation of graft and block copolymers. Waste management, radiation processing, plasma processing, smart polymers.

Books recommended

1. Textbook of Polymer science, F. W. Billmeyer, John Wiley and Sons publication.
2. Principles of polymer chemistry: A. Ravve, Kluwer Academic publications
3. Polymer Chemistry: An Introduction, S. P. Malcolm, Oxford University Press
4. Polymer Science and technology, J. R. Fried, Prentice – Hall.
5. Principles of polymer systems, F. Rodriguez; C.Cohen; C. K. Ober; L. A. Archer, Taylor & Francis
6. Introduction to polymers, R.J. Young; P.A. Lovell, Netron Thornes publications
7. Polymeric materials: Structure - Properties – Applications, W. E., Gottfried, Hanser Gardner Publications
8. Principles of polymer science, P.Bahadur; N.V. Shastri, Narosa publishing house
9. Introductory polymer chemistry, G. Mishra, New age Int. publication.
10. Polymer chemistry and physics of modern materials, J. M. H Cowie; Stancly, Thomas publication.

M.Sc. CHEMISTRY
MEDICINAL CHEMISTRY – II
MCHCCI-411

50 Hours

Unit – I:

QSAR and Drug Design: Durg likeness QSAR parameters, Concept of *in silico* library design through docking studies. Prodrugs, factors governing drug resistance and design of improved drugs with relevant examples like beta lactamase and its inhibitors. Various stages of drug discovery viz., design, synthesis, *in vitro/in vivo* screening, toxicology, ADME studies, clinical studies phases. Brief description of Generic drugs & process development-process technology and up-scaling with example.

The commercial synthetic procedures, classification, mechanism of action, uses and structure activity relationship for selected drugs as included under units II, III and IV shall be covered.

Unit – II:

(a) Sedative hynotics

Pentobarbitone, Allobarbitone

(b) Anticonvulsants

Phenytoin, Trimethadione

(c) Cardiovascular drugs

Beta blockers – Clonidine and Methyl Dopa

ACE inhibitor - Captopril

Unit – III:

(a) Non steroidal anti inflammatory agents

Indomethacin, Ibuprofen, Aspirin

(b) Opoid analgesics

Morphine sulphate, Codeine

(c) Diuretics

Chlorothiazide, Acetazolamide

Unit – IV:

(a) Hypoglycemic agents

Insulin, Tolbutamide

(b) Local Anesthetics

Lignocaine, Procaine

(c) General anesthetics

Cyclopropane, Halothane, Thiopental sodium

Books recommended

1. Introduction to Medicinal Chemistry, A Gringuage,Wiley-VCH

2. Wilson and Gisvold's Textbook of organic medicinal and pharmaceutical chemistry, Edited by Robert F. Doerge.
3. Burgers Medicinal Chemistry and Drug Discovery Vol-1, Ed. M.E. Wolff, John Wiley and Sons
4. Principles of Medicinal Chemistry by W.O. Foye. Varghese publishing house Mumbai
5. The pharmacological basis of therapeutics, L.S. Goodman, A. Gilman
6. The organic Chemistry of drug synthesis, D Lednicer. L.A. mitscher
7. Medicinal Chemistry by D. Srirarm, P. Yogeeswari Published by Dorling Kindersely (India) Pvt. Ltd. Patpargang, New Delhi
8. Introduction to Medicinal Chemistry, A Gringuage, Wiley-VCH
9. An Introduction to Drug Design, S.S. Pandeya and J.R. Dimmock, New Age International.
10. Goodman and Gilman's Pharmacological Basis of Therapeutics, McGraw-Hill.
11. Strategies for Organic Drug Synthesis and Design, D. Lednicer, John Wiley.

M.Sc. CHEMISTRY
LAB COURSE – II
MCHCCI-412

100 hours

The experiments shall be covered from the following practical course:

Preparation of polystyrene using free radical initiators.
Preparation of phenol- formaldehyde resin with natural fibers.
Estimation of molecular weight of polymer using viscometer /gel permeation chromatography.
Preparation of polyacrylamide emulsion polymers.
Preparation of copolymer of styrene/acrylic acid
Preparation of rayon
Preparation of polymer from potato starch
FTIR of PP, Nylon, PET, Acrylic
Crosslinkng of polystyrene with divinylbenzene.
Hydrolysis of acrylic polymers- carboxyl determination
Determination of Aflotoxins by HPLC
Determination of pesticide contamination in fruits and vegetables by GC & HPLC
Determination of DO, BOD and COD of water samples.
Determination of alkalinity, pH, conductivity, hardness, total solids, total dissolved solids (TDS) in given water samples.
Determination of physical and electrochemical parameters of the given soil samples.
Determination of nitrates, nitrites, phosphorous and sulfate in given soil samples.
Screening for PCBs by Perchlorination and GC
Polycyclic aromatic hydrocarbons (PAHs) by Liquid-Liquid Extraction and HPLC with coupled UV and fluorescence detection.

Books recommended

Experimental Methods in Polymer Science, Modern Methods in Polymer Research and Technology, by Toyochi Tanaka, Academic Press, 1999
Environmental Sampling and Analysis: Lab Manual by Maria Csuros, Springer,

**M.Sc. CHEMISTRY
PROJECT
MCHDCE-413**

Marks 100

The project shall comprise of the following three components viz Part A of 50, Part B of 25 and Part C of 25 marks each given as under.

Part A:

Each student will undertake a project work in any industry/institute/research centre during summer vacation under the supervision of an expert from the industry/institute/research centre/with whom the student would be working and under the overall supervision of Head, Department of Chemistry, Jamia Hamdard. After the completion of the project work, each student has to submit a project report by the deadline fixed for the same purpose

Part B:

Each student will make a presentation of the work carried out on the assigned topic followed by viva voce on the date and time fixed for the purpose.

Part C:

Each student will be continuously evaluated for his performance in execution of his or her project work during the entire training period by the supervisor assigned by the department for him to supervise the project work

Discipline centric elective courses: III Semester

M.Sc. CHEMISTRY MEDICINAL CHEMISTRY MCHDCE-304

50 Hours

Unit – I

Drug Design: Development of New Drug, Procedures followed in drug design, Concepts of lead compounds and lead modification: a) Identification of active part: The pharmacophore b) Functional group modification, c) Structure-activity relationship d) Structure modification to increase potency and the therapeutic index: Homologation; Chain branching; Ring-chain transformation; Bioisosterism, Structural Modification to increase oral Bioactivity: Electronic Effect, The Hammett equation, Lipophilicity effects, concepts of prodrugs, soft drugs and drug delivery systems. Theories of drug activity – occupancy theory, rate theory, induced fit theory Concept of drug receptors – elementary treatment of drug-receptor interactions; Physicochemical parameters – lipophilicity, partition coefficient, electronic ionization constants, steric, Shelton and surface activity parameters and redox potentials; Factors affecting modes of drug administration, absorption, metabolism and elimination; Significance of drug metabolism in medicinal chemistry. Various stages of drug discovery viz., design, synthesis, *in vitro/in vivo* screening, toxicology, ADME studies, clinical studies phases.

The commercial synthetic procedures, classification, mechanism of action, uses and structure activity relationship for selected drugs as included under units II, III and IV shall be covered.

Unit – II

(a) Antibiotics

Penicillin, Cephalosporins, Tetracyclines, Macrolides, Streptomycin, Chloramphenicol and Quinolones.

(b) Sulpha drugs

Sulphanilamide, Sulphathiazole, Sulphadiazine and Sulphaacetamide

(c) Antimalarials

Chloroquine phosphate, Primaquine and Mefloquine

(d) Antifungal Agents

Ketoconazole, Griseofulvin

(e) Anthelmintics

Albendazole, Mebendazole

Unit – III

(a) Anti-tubercular

Isoniazid, Rifampicin, Pyrazinamide, and Ethambutol

(b) Anti-neoplastics

Melphalan, Chlorambucil, Cisplatin

(c) Anti-amoebics

Emetine, Metronidazole and Tinidazole

(d) Sedative hypnotics

Pentobarbitone, Allobarbitone

(e) Anticonvulsants

Phenytoin, Trimethadione

Unit – IV

(a) Cardiovascular drugs

Beta blockers – Clonidine and Methyl Dopa

ACE inhibitor – Captopril

(b) Non steroidal anti inflammatory agents

Indomethacin, Ibuprofen, Aspirin

(c) Hypoglycemic agents

Insulin, Tolbutamide

(d) Local Anesthetics

Lignocaine, Procaine

(e) General anesthetics

Cyclopropane, Halothane, Thiopental sodium

Books recommended

1. Introduction to Medicinal Chemistry, A Gringuage, Wiley-VCH
2. Wilson and Gisvold's Textbook of organic medicinal and pharmaceutical chemistry, Edited by Robert F. Doerge.
3. Burgers Medicinal Chemistry and Drug Discovery Vol-1, Ed. M.E. Wolff, John Wiley and Sons
4. Principles of Medicinal Chemistry by W.O. Foye. Varghese publishing house Mumbai
5. The pharmacological basis of therapeutics, L.S. Goodman, A. Gilman
6. The organic Chemistry of drug synthesis, D Lednicer. L.A. mitscher
7. Medicinal Chemistry by D. Srirarm, P. Yogeeswari Published by Dorling Kindersely (India) Pvt. Ltd. Patpargang, New Delhi
8. Introduction to Medicinal Chemistry, A Gringuage, Wiley-VCH
9. An Introduction to Drug Design, S.S. Pandeya and J.R. Dimmock, New Age International.
10. Goodman and Gilman's Pharmacological Basis of Therapeutics, McGraw-Hill.
11. Strategies for Organic Drug Synthesis and Design, D. Lednicer, John Wiley.

M.Sc. CHEMISTRY
CATALYSIS AND GREEN CHEMISTRY
MCHDCE-305

50 Hours

Unit-I

Principles of Sustainable and Green Chemistry: Basic principles of green chemistry, Tools of green chemistry, Green Chemistry and Industry, Waste Minimisation and Atom Economy, Some inherently atom economic and uneconomic reactions. Reduction of materials use- Concept of sustainability, Reduction of non-renewable raw material use, Catalytic solutions, Process intensification, Reduction of energy requirement, Some energy efficiency improvements, Alternative energy sources, Reduction of risk and hazard, Inherently safe design, Alternative solvents.

Unit-II

Solvent free Chemistry: Organic Synthesis in Solid State; Alternative Solvents: Water; Supercritical fluids- Supercritical CO₂ as a replacement for organic solvents, Extraction of Natural Products; Multiphase and single phase processes using supercritical CO₂ as a reaction and separation phase, Simultaneous use of supercritical CO₂ as reaction medium and reagent; Renewable Solvents; Ionic Liquids- reactions in acidic and neutral ionic liquids; Fluorous Solvents- biphasic concept, synthesis of fluorous compounds, fluorous extraction, fluorous synthesis, fluorous reagents; Liquid Polymers: PEG, PPG, Poly(dimethylsiloxane)

Unit III

Sonochemistry in Chemical Synthesis: Sonochemical reactions: Substitution, addition, oxidations, reductions, esterification, hydrolysis, and coupling reactions, Ultrasonic preparation of micro- and nanostructured materials.

Approaches to Microwave-assisted Organic Chemistry: solvent-free methods, methods with solvents, Metal-catalysed Processes, Enzymatic Processes.

Photochemistry: Photons as Clean Reagents, Reduced usage of reagents, Lower reaction temperatures, Control of selectivity

Unit IV

Catalysis: Solid Acid Catalysts- Zeolite-based solid acid catalysts, Heteropolyacid-based solid acid Catalysts, Sulfated zirconia, Ion-exchange resins, Acidic and pillared clays; Micelle-templated Silicas as Catalysts: Catalytic Applications, Oxidation catalysis, Base catalysis (other than oxidations), Enantioselective catalysis

Books recommended

1. Green Chemistry- Theory and Practice by Paul T. Anastas, John C. Warner, Oxford University press, 1998.
2. Methods and reagents for green chemistry-An Introduction, Pietro Tundo, Alvise Perosa, Fulvio Zecchini, John Wiley & Sons, Inc., 2007
3. Green Solvents For Chemistry-Perspectives and Practice by William M. Nelson, Oxford University Press, Inc. 2003
4. Alternative Solvents for Green Chemistry by Francesca M. Kerton, The Royal Society of Chemistry, 2009
5. Green chemistry and the ten commandments of sustainability by Stanley E. Manahan, ChemChar Research, Inc., 2006

M.Sc. CHEMISTRY
METHODS OF CHEMICAL ANALYSIS
MCHDCE-306

50 Hours

Unit I

Atomic Spectroscopy: Introduction, basic principle of atomic absorption, methodology, sample preparation, flame, electrothermal atomization, hydride methods, principle of atomic emission spectroscopy. Instrumentation of ICP spectrometer-sequential and simultaneous elemental analysis

Unit II

Electroanalytical methods: Classification of electroanalytical methods, basic principle of pH metric, potentiometric and conductometric titrations. Techniques used for the determination of equivalence points. Techniques used for the determination of pK_a values.

Unit III

Electrophoretic Techniques: Principle, equipment and process, Agarose gel electrophoresis, horizontal and vertical gel electrophoresis, electrophoresis techniques, Isoelectric focusing, capillary electrophoresis and application of electrophoresis in analysing macromolecules.

Centrifugation: Introduction, Basic Principle of sedimentation, Types, care and safety of centrifuges, Preparative centrifugation, Analytical centrifugation, Ultracentrifugation

Unit IV

X-ray Methods: Production of x-ray spectra, absorption of x-rays, analysis by absorption, absorption edge analysis, absorption apparatus, determination of molecular structure by X-ray diffraction, crystal morphology, lattice and unit cells, kinds, space lattice, planes or faces of cubic systems, labeling the planes, the Miller indices, spacing of the planes, X-ray crystallography, the powder methods, the rotating crystal methods.

Books recommended

1. Instrumental Methods of Analysis, 7th edn., H.H. Willard, L.L. Merritt, Jr., J.A. Dean and F.A. Settle, Jr., C.B.S. Publishers and Distributor, 1986, Tata McGraw (New Delhi)
2. Instrumental methods of Chemical Analysis, 5th edn., G.W. Ewig.
3. Instrumental Methods of Analysis by G.D. Christian and C.N. Reilly
4. Principle of Instrumental Methods of Analysis; D.A. Stoog, D.M. West and F.J. Holler, Sounders College Publishing New York, 2001.
5. Ionic Equilibria in Analytical Chemistry; Freiser and Fernando
6. Chemical Analysis, H.A. Laitinen

Open Elective Course: III Semester

M.Sc. CHEMISTRY ENVIRONMENTAL CHEMISTRY MCHOE-307

50 lectures

Unit I

Composition of atmosphere; chemical and photochemical reaction cycles of C, N, P, S and O.

Air pollutants - CO, CO₂, ozone, CFC; ozone depletion; global warming

Unit II

Harmful effects of pollutants on living and non-living species;

Analytical methods for monitoring air pollutants; international and national standards.

Unit III

Physical, chemical and biological water quality parameters; their assessment.

Water pollution; water pollutants; toxicity aspects; international and national standards; control.

Unit IV

Water treatment processes: aeration, solid purification nanofiltration, chemical treatments, reverse osmosis, desalination.

Water table maintenance & harvesting methods.

Industrial pollution: Sugar, drug, paper and pulp sectors, thermal power plants. Disposal of wastes and its management. Chemical solutions to environmental problems, principles of decomposition, biodegradability, better industrial processes.

Books recommended

- Environmental Chemistry, S. E. Manahan, Taylor & Francis Ltd
- Basic Concepts of Environmental Chemistry, D.W. Connell, CRC-Press
- Environmental Chemistry: A Global Perspective, G.W. Vanloon; S. J. Duffy , Oxford Univ Pr (Sd)
- Introduction To Environmental Chemistry, J. B. Reid, Blackwell Science Ltd
- Chemistry of the Environment, T. G. Spiro; W. M. Stigliani, Prentice Hall publication.
- Environmental Chemistry, G. W Duffy; J. Stephen, Oxford Higher Education publication
- Environmental Chemistry, C. Baird; M.Cann, W. H. Freeman

Discipline Centric Elective Course- IV Semester

M.Sc. CHEMISTRY POLYMER CHEMISTRY MCHDCE-404

50 Hours

Unit I

Structure, classification and nomenclature of polymers: Physical properties of the polymers- Amorphous and crystalline arrangements-Amorphous state, Elasticity, Crystallinity, thermal transitions, effect of chemical structure on physical properties, solubility of polymers, molecular weight and molecular weight distribution, Steric arrangement

Unit II

Chain growth polymerization: Free radical polymerization process, kinetics, initiators, efficiency of initiators, chain growth, steric, polar and resonance effects in the propagation reaction, termination of polymeric reactions, chain transfer, control of molecular weight, inhibitors and retarders, Effect of reaction medium and temperature on chain polymerization, ceiling temperature, Autoacceleration

Ionic chain growth polymerization: Cationic polymerization- Kinetics, Initiators, propagation, and termination reactions. Anionic polymerization- Kinetics, Initiators, propagation, and termination reactions. Coordinated anionic polymerization, Heterogenous and homogenous Ziegler Natta catalysts

Step growth polymerization: Mechanism, kinetics and statistics of linear step growth polymerization, Carother's equation, Co-polymerisation- mechanisms, kinetics, Copolymer equation, monomer reactivity ratio, graft polymerization and block copolymerization. Ring opening polymerization, kinetics, cationic, anionic and hydrolytic polymerization of lactams.

Unit III

Characterization of polymers: molecular weight and molecular distribution: molecular weight determination by osmometry, light scattering, viscometry and gel permeation chromatography, end group analysis, TGA, DSC and DMA with suitable examples.

Polymer processing: classification of polymer processing, extrusion and extruders, calendering, film blowing, injection moulding, blow moulding, vacuum forming, rotational, transfer and compression moulding, fibre spinning, polymer additives.

Unit IV

Industrial polymers: polyethylene, polypropylene, PTFE, PMMA, polyacrylonitrile, nylons. polyethylene terephthalate, polycarbonates, natural rubber, polyisoprenes, rubbers derived from butadiene, cellulose and related polymers, phenol-formaldehyde polymers, urea formaldehyde resin, polyurethanes.

Books recommended

1. Textbook of Polymer science, F. W. Billmeyer, John Wiley and Sons publication.
2. Principles of polymer chemistry: A. Ravve, Kluwer Academic publications
3. Polymer Chemistry: An Introduction, S. P. Malcolm, Oxford University Press
4. Polymer Science and technology, J. R. Fried, Prentice – Hall.
5. Principles of polymer systems, F. Rodriguez; C. Cohen; C. K. Ober; L. A. Archer, Taylor & Francis
6. Introduction to polymers, R.J. Young; P.A. Lovell, Netron Thornes publications
7. Polymeric materials: Structure - Properties – Applications, W. E., Gottfried, Hanser Gardner Publications
8. Principles of polymer science, P. Bahadur; N.V. Shastri, Narosa publishing house
9. Introductory polymer chemistry, G. Mishra, New age Int. publication.
10. Polymer chemistry and physics of modern materials, J. M. H. Cowie; Stancly, Thomas publication.

M.Sc. CHEMISTRY
BIOORGANIC AND BIOINORGANIC CHEMISTRY
MCHDCE-405

50 Hours

Unit – I

Enzymes: Introduction and historical perspective, chemical and biological catalysis, remarkable properties of enzymes like catalytic power, specificity and regulation. Nomenclature and classification, extraction and purification. Fisher's lock and key and Koshland's induced fit hypothesis, concept and identification of active site by the use of inhibitors, affinity labeling and enzyme modification by site-directed mutagenesis. Enzyme kinetics, Michaelis-Menten and Lineweaver-Burk plots, reversible and irreversible inhibition.

Mechanism of Enzyme Action: Transition-state theory, orientation and steric effect, acid-base catalysis, covalent catalysis, strain or distortion. Examples of some typical enzyme mechanisms for chymotrypsin, ribonuclease, lysozyme and carboxypeptidase A.

Enzyme Applications in Organic Synthesis: Introduction, optical rotation and enantiomeric excess, general aspect of enzyme catalysts, hydrolysis and formation of C-O bonds, hydrolysis of C-N bond, epoxide and nitrile hydration, oxido-reductases, carbon-carbon bond forming reactions, lyases, immobilization of enzymes/cells, industrial applications of immobilized enzymes and cells

Unit-II

Kinds of Reactions Catalysed by Enzymes: Nucleophilic displacement on a phosphorus atom, multiple displacement reactions and the coupling of ATP cleavage to endergonic processes. Transfer of sulphate, addition and elimination reactions, enolic intermediates in isomerization reactions, β -cleavage and condensation, some isomerization and rearrangement reactions. Enzyme catalyzed carboxylation and decarboxylation.

Co-Enzyme Chemistry: Cofactors as derived from vitamins, coenzymes, prosthetic groups, apoenzymes. Structure and Biological functions of coenzyme A, thiamine pyrophosphate, pyridoxal phosphate, NAD^+ , FMN, FAD, lipoic acid, vitamin B_{12} . Mechanisms of reactions catalyzed by the above cofactors.

Unit III:

Metal Ions in Biological Systems: Essential and trace metals in biological system, classification and application; Deficiency/ excess and treatment; antagonistic effect of elements and its remedy.

Na^+/K^+ Pump: Roles of metals ions in biological processes.

Transport and Storage of Dioxygen: Heme proteins and oxygen uptake; structure and function of hemoglobin, myoglobin, oxygen transport in mammals, importance of Fe^{2+} Bohr's effect, Perutz mechanism. hemocyanins and hemerythrin; model synthetic complexes of iron, cobalt and copper; Vaska compound.

Unit IV:

Electron Transfer in Biology: Structure and functions of metalloproteins in electron transport processes – cytochromes and iron-sulphur proteins; synthetic models.

Nitrogenase: Biological nitrogen fixation, molybdenum nitrogenase, spectroscopic and other evidence, other nitrogenase model systems.

Books Recommended:

1. Principles of Bioinorganic Chemistry, S.J. Lippard and J.M. Berg, University Books.
2. Bioinorganic Chemistry, I. Bertini, H.B. Gray, S.J. Lippard and J.S. Valentine, University Science Books.
3. Inorganic Biochemistry, Vols. I and II. Ed., G.L. Eichhorn, Elsevier.
4. Progress in Inorganic Chemistry, Vols. 18 and 38 ed. J.J. Lippard, Wiley.
5. Bioorganic Chemistry: A Chemical Approach to Enzyme Action, Hermann Dugas and C. Penny, Springer-Verlag
6. Understanding Enzymes, Trevor Palmer, Prentice Hall
7. Enzyme Chemistry: Impact and Applications, Ed. Collin J. Suckling, Chapman and Hall
8. Enzyme mechanisms, Ed. M.I. Pajonk, A. Williams, RSC
9. Fundamentals of Enzymology, N.C. Price, L. Strevens, Oxford University Press.
10. Immobilized Enzymes: An Introduction and Applications in Biotechnology, Michael D. Trevan, John Wiley
11. Enzymatic Reaction Mechanisms, C. Walsh, W.H. Freeman
12. Enzymes- Structure and Mechanism, A. Fersht, W.H. Freeman
13. Biochemistry: The Chemical Reactions of the Living Cells, D. E. Metzler, Academic Press

M.Sc. CHEMISTRY
Molecular Modelling & Drug Design
MCHDCE-406

50 Hours

Unit I

Introduction to Molecular Modelling: Introduction - Useful Concepts in Molecular Modelling : Coordinate Systems. Potential Energy Surfaces. Molecular Graphics. Surfaces. Computer Hardware and Software. The Molecular Modelling Literature.

Quantum chemistry: Single- and multiple electron systems. Ab initio-methods, Hartree-Fock equations, gaussian basis sets. Orbitals, calculation of partial charges, practical program usage.

Unit II

Molecular force fields: Bonds, angles, torsions. Electrostatics and van der Waal forces, parameterisation from experiments or quantum chemistry. Effective pair potentials, hydrogen bonds. Computation of molecular properties and limitations, examples of commonly used force fields.

Unit III

Energy landscapes: Minimizations, algorithms, normal modes, transition states and reaction pathways.

Simulation methods: Molecular dynamics, equilibration, thermodynamical properties from simulations, stochastic dynamics, energy conservation. Monte Carlo methods and conformational analysis.

Unit IV

Bioinformatics: Sequence analysis, protein structure, homology modeling, 3D structure prediction from sequence, chemoinformatics, combinatorial databases.

Advanced applications: Free energy calculations from simulations, free energy of solvation, chemical reactions, molecular docking, modern drug design with simulations and quantum chemistry.

Books Recommended:

Leach, A. R. *Molecular modelling - principles and applications*, 2nd ed., ISBN 0-582-38210-6
J.M.Haile, *Molecular Dynamics Simulation Elementary Methods*, John Wiley and Sons, 1997.
Satya Prakash Gupta, *QSAR and Molecular Modeling*, Springer - Anamaya Publishers, 2008.

Open Elective Course – IV semester

M.Sc. CHEMISTRY Chemistry in Nanoscience MCHOE-407

50 Hours

Unit-I

NANOPARTICULATE DRUG-DELIVERY SYSTEMS

Methods of Measurements and characterization of nanomaterials - transmission electron microscopy, scanning electron microscopy, scanning probe techniques (scanning probe microscopy), optical tweezers (single-beam gradient trap). Manufacture of nanomaterials - bottom-up manufacturing, top-down manufacturing

Unit-II

POLYMER-BASED NANOPARTICULATE DRUG-DELIVERY SYSTEMS

Drug-delivery systems - lipid-based colloidal nanodrug-delivery systems, solid-lipid nanoparticle system, nanoparticulate polymeric micelles as drug carriers, polymeric micelles and solubilization of drugs, polymeric micelles and reticuloendothelial system, recent trends in polymeric micelles research. Hydrogel-based nanoparticulate drug-delivery systems - Dendrimer-based drug-delivery systems,

Unit-III

DIVERSE AND EMERGING TRENDS IN NANOTECHNOLOGY APPLICATIONS

Biological analysis and discovery, nanoparticle tagging, nanostructured materials, single-molecule detection, protective nanoparticles against pathogens, nanotubes and cellular manipulation, antibody-coated nanospheres, nanocrystallites, nanohybrids, nanocontainer technology, electrospun nanofibers as drug-delivery systems, future directions.

Unit-IV

ROLE OF NANOTECHNOLOGY IN THE DEVELOPMENT OF NANOMEDICINE

Role of nanotechnology in molecular diagnostics, nanoparticles for molecular diagnostics, gold nanoparticles, quantum dots, magnetic nanoparticles, role of nanotechnology in drug discovery, nanoparticles for drug discovery, use of gold nanoparticles for drug discovery, use of quantum dots for drug discovery

Books recommended

1. Nanoparticulate Drug Delivery System by Michael Deleers
2. Handbook of Nanobook by Gary Wiederrecht
3. Nanoparticles: Synthesis, Stabilization, Passivation, and Functionalization by T. Alan Hatton
4. Polymeric Drug Delivery Systems by James Swarbrick