M.Sc. Chemistry
Scheme & Syllabus

Semester 1

Course Code	Course Title	Load Allocation			Marks Distribution			Credits
		L	T	P	External	Internal	Total	
MSCH-21101	Inorganic Chemistry-I	4	1	0	100	50	150	5
MSCH-21102	Organic Chemistry-I	4	1	0	100	50	150	5
MSCH-21103	Basic Biological Chemistry/ Mathematics in Chemistry	4	1	0	100	50	150	5
MSCH-21104	Physical Chemistry	4	1	0	100	50	150	5
MSCH-21105	Inorganic Chemistry Lab-I	0	0	6	100	50	150	3
MSCH-21106	Organic Chemistry Lab-I	0	0	6	100	50	150	3
Total		16	4	12	600	300	900	26

Semester 2

Course Code	Course Title	Load Allocation			Marks Distribution			Credits
		L	T	P	External	Internal	Total	
MSCH-21201	Organic Chemistry-II	4	1	0	100	50	150	5
MSCH-21202	Symmetry and Group Theory	4	1	0	100	50	150	5
MSCH-21203	Spectroscopyï I	4	1	0	100	50	150	5
MSCH-21204	Quantum Chemistry	4	1	0	100	50	150	5
MSCH-21205	Physical Chemistry Lab	0	0	6	100	50	150	3
MSCH-21206	Organic Chemistry Lab-II	0	0	6	100	50	150	3
Total		16	4	12	600	300	900	26

Semester 3

Course Code	Course Title	Load Allocation			Marks Distribution			Credits
		L	T	P	External	Internal	Total	
MSCH-21301	Inorganic Chemistry-II	4	1	0	100	50	150	5
MSCH-21302	Spectroscopy-II	4	1	0	100	50	150	5
MSCH-21303	Computational Skills and Simulations in Chemistry	4	1	0	100	50	150	5
MSCH-21304	Polymers	4	1	0	100	50	150	5
MSCH-21305	Computational Skills and Simulations in Chemistry Lab	0	0	6	100	50	150	3
MSCH-21306	Inorganic Chemistry Lab-II	0	0	6	100	50	150	3
Total		16	4	12	600	300	900	26

Semester 4

Course Code	Course Title	Load Allocation			Marks Distribution			Credits
		L	T	P	External	Internal	Total	
MSCH-21401	Photochemistry	4	1	0	100	50	150	5
MSCH-21402	Environmental Chemistry	4	1	0	100	50	150	5
MSCH-21403	Analytical principles and Instrumental Method of Analysis	4	1	0	100	50	150	5
MSCH-21XXX	Elective*	4	1	0	100	50	150	5
MSCH-21404	Advanced Chemistry Lab	0	0	6	100	50	150	3
Total		16	4	6	500	250	750	23

***Elective- MSCH-21405 Nanochemistry / MSCH-21406 Medicinal Chemistry / MSCH-21407 Surface Chemistry, Adsorption and Catalysis**

MSCH-21101 Inorganic chemistry-I

Internal Marks: 50 **L T P**
External Marks: 100 **4 1 0**
Total Marks: 150

Course Objective:

1. To understand Principles of Molecular Orbital Theory and VSEPR theory completely.
2. To acquire full knowledge of main group chemistry and group 12 elements.
3. To know the structures of ionic solids.
4. To develop an understanding of the inorganic chemistry of elements with respect to their oxidation and reduction.

1. Principles

Molecular structure and bonding. A review of Lewis structures including formal charges and VSEPR model. Molecular orbital theory of homo- and heteronuclear diatomic molecules. Molecular orbital theory of solids. Periodicity and related concepts. Chemical forces. (7)

2. Chemistry of s-block metals

Hydrides, halides, oxides, peroxides, superoxides, suboxides, hydroxides, oxoacid salt complexes, crowns and crypts of alkali metals and coordination complexes of alkaline earth metals. (10)

3. Chemistry of p–block elements

Boranes, bonding in boranes, topology of boranes, synthesis and reactivity. Carboranes and metallocarboranes, borazine and boron nitride. Chemistry of aluminum halides, aluminum alkyls. Low oxidation state aluminium compounds. Organosilicon compounds. Sillicates and aluminosilicates. Low-valent silicon compounds, silylenes and $R3Si^{+}$, Polysilanes. Phosophazenes, cyclophosphazenes, polyphosphazenes and the polymers derived from them. (10)

4. Chemistry of group 12 elements

Halides & oxygen compounds, chalcogenides & related compounds, low-valent compounds. Formation of coordination complexes. (5)

5. Solid state

Close-packing of solids, types and structures of ionic solids; radius ratio rules; lattice energy; Bornï Haber cycles, defects in solids and properties of solids arising out of defects in structures, Perovskite structures, high Tc superconductors. (7)

6. Oxidation and reduction

Reduction potentials, redox stability in water , diagrammatic presentation of potential data, acids and bases, Various definitions including HSAB principles, Thermodynamic acidity parameters, solvents as acids and bases. (6)

Suggested Books:

1. W. Henderson, Main Group Chemistry, Royal Society of Chemistry, UK, 2000.
2. J. E. Huheey et. al, Inorganic Chemistry, Principles of Structure and Reactivity, Fourth edition, Pearson Education, India, 2006.
3. J. D. Lee, Concise Inorganic Chemistry, Fifth edition, Wiley India Pvt, Ltd. 2008.
4. Norman Greenwood, Andrew Hughes, Mark Fox, Keith Dillon, Kenneth Wade, Chemistry of Elements, Elsevier, 2011.
5. Peter Atkins, Tina Overton, Shriver and P. W. Atkinsô Inorganic Chemistry, 5th edition Oxford University Press, Oxford, 2009.
6. F. Albert Cotton, Carlos A. Murillo, Manfred Bochmann, Russell N. Grimes, Advanced Inorganic Chemistry,6th edition, Wiley-Interscience, 1999.

MSCH-21102 Organic chemistry-I

Internal Marks: 50 **L T P**
External Marks: 100 **4 1 0**
Total Marks: 150

Course Objective:

1. To understand different types of organic synthesis.
2. To understand use of various reagents in organic synthesis.
3. To understand asymmetric synthesis and characterize the compounds synthesized.

1. General Introduction to organic synthesis, types of organic synthesis: retrosynthesis, disconnection, Linear and convergent synthesis, synthons, synthetic equivalents, umpolung of reactivity and protective groups, protection and deprotection of general functional groups, functional group interconversions, applications of green chemistry to organic synthesis. (12)

2. Use of following reagents in Organic synthesis and functional group transformations; compounds of Mg, Li, Cu, B, Si and P in organic synthesis, Gilmanôs reagent, lithium diisopropylamide (LDA), dicyclohexylcarbodiimide (DCC), 2,3-Dichloro-5,6-dicyano-1,4-benzoquinone (DDQ), trimethylsilyl iodide, tri-n-butyltin hydride, osmium tetroxide, selenium dioxide. Phase transfer catalysts, crown ethers and Merrifield resin, Wilkinsonôs catalyst, Baker yeast, ionic liquids, water. (11)

3. Asymmetric synthesis: Chiral auxillaries, methods of asymmetric induction-substrate, reagent and catalyst controlled reactions, determination of enantiomeric purity by GC, HPLC, NMR etc., enantio-discrimination, resolution- optical and kinetic, chiral phase transfer catalysis, chiral quaternary ammonium salts, asymmetric proton catalysis, asymmetric acyl transfer reactions. (11)

4. General methods of preparation and reactions of indene, fluorine, anthracene and phenanthrene, three-membered, four-membered, five-membered and six-membered heterocyclic compounds: synthesis and reactions of oxiranes, thiiranes, azetidines, aziridines, oxetanes, thietanes, pyrrole, pyrrolidine, furan, tetrahydrofuran, pyrylium salts, pyrones, pyridinium and thiopyrylium salts, pyridones, quinolizinium and benzopyrylium salts, coumarins and chromones. (11)

Suggested Books:

1. Willis Christine and Wills Martin, Organic Synthesis, Oxford University Press, 1995.

2. Corey E.J., X.M. Cheng, The logic of Chemical Synthesis, Wiley Interscience, 1995.
3. Thomas S.E., Organic Synthesis: The roles of Boron and Silicon, Oxford University Press, 1992.
4. Jenkins Paul R., Organometallic Reagents in Synthesis, John Wiley, 1994.
5. Mackie R.K., Smith D.M., Guide Book to Organic Synthesis, 2nd edition, Longman, 1995.
6. Acheson R.M., An Introduction to the Chemistry of Heterocyclic Compounds, Wiley, 3rd edition, New York, 1976.
7. Michael B. Smith, Jerry March, March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, (6th Edition), Wiley-Interscience, 2007.
8. Carey F.R., Sunberg R.J., Advanced Organic Chemistry, 5th edition, Springer, 2007.
9. Devies Stephen G., Organotransition Metal Chemistry: Applications to Organic Synthesis, Pergamon Press (1994).
10. Morrison J.D. (eds.), Asymmetric Synthesis: Vol.1-5; Academic Press, 1992.
11. Aitken R.A., Kilenyi S.N., Asymmetric Synthesis

MSCH-21103 Basic Biological Chemistry

External Marks: 100 **L T P**
Internal marks: 50 **4 1 0**
Total Marks: 150

Course Objective:

1. To understand detailed structures of proteins & nucleic acids.
2. To understand role of enzymes.
3. To understand detailed mechanism and functions of carbohydrates.

1. Human biology and cell structure

Characteristics of living organisms, nutrition, Digestion, Respiration, Body fluids and Circulation, Excretion, Skeleton system & muscle, Nervous, Physiology of high altitude. Structure of prokaryotic & eukaryotic cells, Intrcellular organelles and their functions, Comparison of plant and animal cells. Overview of metabolic process - catabolism and Anabolism. ATP - the Biological energy currency. Cell division stages of mitosis & meiosis. Significance of cell division and fertilization. (12)

2. Carbohydrates

Monosaccharides, structure & functions of important derivatives of monosaccharides(Enantiomers, Epimers, Hemiacetal, Hemiketalepanomers). O-glycosidic bond disaccharide & Polysaccharides. Reducing and non-reducing sugars. Structural Polysaccharides - cellulose and chitin. Storage Polysaccharides - starch and glycogen. Structure and Biological functions. Carbohydrate metabolism - Kreb's Cycle, glycolysis, glycogenesis and glycogenolysis, gluconeogenesis, Pentose phosphate Pathway. (11)

3. Lipids

Fatty acids, essential fatty acids, structure and function. Storage lipids. Triacyl glycerols. Structural lipids-phospholipids, Glycolopids with special emphasis on blood groups. Archae bacterial ether lipids. Lipoproteins ð composition and function. (6)

4. Nucleic acids

Purines and Pyrimidine bases, base pairing via H-bonding. Structure of ribonuclic acids (RNA) and deoxyribonucleic acids (DNA), double helix model of DNA and forces responsible for holding it, Chemical and enzymatic hydrolysis of Nucleic acids, Replication and translation. (6)

5. Proteins and enzymes

Configuration properties of amino acids, Structural and functional classification of proteins. Purification of proteins and amino acid sequence determination, peptide bond. Primary, secondary tertiary and quaternary structures of proteins, Ramachandran plot. Structure and functions of hemoglobin. Classification and nomenclature of enzymes. Mechanism & kinetics of enzymatic reactions. Michaelis Menton model, enzyme inhibition. Kinetics of competitive and non-competitive enzymatic inhibition. Isozymes allosteric enzymes. (10)

Suggested Books:

1. L. Stryer, Biochemistry, W.H. Freeman & Company, 4th Edition, 1995.
2. D. Voet and J.G. Voet, Biochemistry, John Wiley & Sons, 2nd Edition, 1995.
3. Michael D. Trevan, Immobilized Enzymes: An introduction and application in Biotechnology, John Wiley, 1980.

MSCH-21103 Mathematics in Chemistry

External Marks: 100 **L T P**
Internal marks: 50 **4 1 0**
Total Marks: 150

Course Objective: To understand the basic concepts of mathematics.

1. Matrix Algebra
Addition and multiplication, determinants, inverse, adjoint and transpose of matrices, special matrices (Symmetric, skew-symmetric, Hermitian; skew- Hermitian, unit, diagonal, unitary etc.) and their properties. Matrix equations: Homogeneous, non-homogeneous, linear equations and conditions for the solution, linear dependence and independence. Cayley Hamilton theorem, matrix eigenvalues and eigenvectors. (10)

2. Differential Calculus
Functions, continuity and differentiability, rules for differentiation, applications of differential calculus including maxima and minima. Functions of several variables, partial differentiation, Euler's theorem co-ordinate transformations (e.g. cartesian to spherical polar). (12)

3. Integral calculus
Basic rules for integration, integration by parts, partial fraction and substitution definite integrals and its properties. (10)

4. Elementary Differential Equations
Variables - separable and exact, first order differential equations. Homogeneous, exact and linear equations. (13)

Suggested Books:
1. Mathematics for Chemistry, Doggett and Sucliffe, Longman.
2. Basic Mathematics for Chemists, Tebbutt Wiley.
3. Higher Engineering Mathematics, B. S. Grewal (Khanna Pub.)
4. Mathematics by R.D. Sharma, Dhanpat Rai Publications, New Delhi.
5. Differential Calculus by Santi Narayan, S.Chand Publications.
6. Integral Calculus by Santi Narayan, S.Chand Publications.
7. Mathematical Preparation for Physical Chemistry, F. Daniels, McGraw Hill.

MSCH-21104 Physical Chemistry

External Marks: 100 **L T P**
Internal marks: 50 **4 1 0**
Total Marks: 150

Course Objective:

1. To understand the laws of thermodynamics.
2. To study the reaction rates of different order reactions.
3. To study the various aspects of electrochemistry.

1. Thermodynamics

Concepts involved in first and second law of thermodynamics, Entropy, chemical potential and free energy . Maxwellõs relations, Partial molar properties and their significance. Concept of activity and fugacity and their determination. Nernst heat theorem, third law of thermodynamics.

General introduction: Phase space, microstates, macrostates, thermodynamic probability. Thermodynamic probability and entropy. Brief introduction to different types of statistics (Maxwell - Boltzman, Bose ï Einstein and Fermi - Dirac statistics). Ensemble concept. Canonical, grand canonical and microcanocical ensembles. Stirling approximation. Maxwell-Boltzmann statistics. Partition functions: Expressions of translational, rotational, vibrational and electronic and nuclear partition functions. (16)

2. Chemical Kinetics

Principle of detailed balancing (simple idea only), Effect of temperature on reaction rates. Collision theory of reaction rates (detailed), preliminary idea of transition state theory, Lindemann theory of Unimolecular reactions. Opposing and consecutive reactions. Static, flow and relaxation methods of measurement of reaction rates. Kinetics of fast reaction. preliminary idea of inner sphere and outer sphere reactions of transition metals.

Homogeneous and heterogeneous catalysis, Michaelis-Menten mechanism for enzyme catalysis, autocatalysis and oscillatory reactions (general introductions only). (10)

3. Electrochemistry: Mean ionic activity co-efficient of electrolyte. Debye ï Huckel theory. Precise determination of dissociation constants of weak electrolytes ï emf and conductometric method. Debye Huckel theory of strong electrolytes, Onsagar conductance equation. Irreversible electrode processes: Polarography and overvoltage. Polarographic cell assembly, merits of dropping mercury electrode. Basic principle of cyclic voltametry and coulometry only. (10)

4. Miscellaneous Topics

Molecular Structure: Dielectric polarization, Debye ï Langevin equation, dipole moment determination and applications, intermolecular forces and their contribution to intermolecular potential.

Fluid Mechanics: Fundamental principles of fluid mechanics, Newtonian and Non-Newtonian fluids. Stream line and turbulent flow.

Refractories: Refractory materials: Nomenclature, classification-acidic, basic and neutral refractories, important properties and uses. (9)

Suggested Books:

1. Silbey, Alberty, et.al., Physical Chemistry, 4th Edition, Wiley India Pvt. Ltd., 2006.
2. Atkins, P.W., Julio de Paula, Physical Chemistry, 8th edition, ELBS, 2006.
3. Chandra, A.K, Introductory Quantum Chemistry, 4th edition, Tata McGraw Hill, 2004.
4. Laidler, Keith J., Chemical Kinetics, 3rd edition, Harper & Row, Publishers, New York, 1987.
5. Young, R.J; Lovell, P.A., Introduction to Polymers, 2nd edition, Chapman and Hall, 1991.
6. Flory, P.J., Principles of Polymer Chemistry, 1st edition, Asian Book Private Ltd., 2006.
7. Crow, D.R., Principles and Applications of Electrochemistry, 4th edition, Chapman and Hall, London, 1994.

MSCH-21105 Inorganic Chemistry Lab-I

External Marks: 100 **L T P**
Internal marks: 50 **0 0 6**
Total Marks: 150

Course Objective:

1. To know skills of using various glass wares and apparatus and chemicals used in synthetic inorganic chemistry.
2. To improve the environment of the laboratory and health of the students.
3. To know the chemistry principles applied in the qualitative analysis.
4. To understand various techniques of salt analysis.

1. Working in Chemistry Lab

Introduction ï Personal protection ï Nature of Chemicals ï Toxic, Corrosive, Explosive, Inflammable, Carcinogenic, other hazardous chemicals ï Safe storing and handling of chemicals ï Disposal of chemical wastes ï Glassware ï Handling of Glassware ï Handling of different types of equipments like Bunsen burner, Centrifuge, Gibbôs Apparatus, etc. ï Ventilation facilities ï Philosophy of Lab Safety ï First-Aid techniques ï General work culture inside the chemistry lab.

2. Preparation of coordination compounds, their purification by chromatography, elemental analyses (S, Halogen, C, H, N), M.W. determination (Rast method) and elucidation of structures by physical methods (UV, IR, NMR, magnetic susceptibility)

(a) Synthesis of Tris(acetylacetonato)manganese (III), Mn(acac)3 and their characterization.

(b) Synthesis and Characterization of Hexamminechromium (III) nitrate $[Cr(NH3)_6](NO_3)_3$ using magnetic susceptibility balance (MSB) and infra red spectroscopy IR (Green Preparation).

(c) Synthesis of Iron (III) dithiocarbamate and its characterization using magnetic succeptibility balance (MSB) and infra red spectroscopy (IR).

(d) Synthesis and characterization of nitro- and nitritopentamminecobalt (III) chlorides using infra red spectroscopy (IR).

(e) Synthesis of hexamminecobalt(III) chloride and pentammineaquocobalt(III) chloride.

(f) Synthesis of cis- and trans- potassiumdioxalatodiaquochromate(III).

(g) Aquation of trans-dichlorobis(1,2-diaminoethane)cobalt(III) chloride.

(h) Synthesis and resolution of tris(ethylenediamine)cobalt(II) ion.

(i) Synthesis of Hexaamminenickle(II) chloride and estimation of Ni(II) in the complex by gravimetry and volumetry.

(j) Synthesis of tris(acetylacetanonato)iron(III).

(k) Synthesis and reactivity of organocobaloximes.

(l) Synthesis of acetylferrocene and its purification by column chromatography.
(m) Synthesis of ferrocene carboxylic acid.

3. Synthesis of green reagents:

Green Chemistry: Introduction, principles of green chemistry, some green reagents.

a) Tetrabutylammonium tribromide (TBATB) and its applications.
b) Ionic liquid, 1-methyl-3-pentyl-imidazolium bromide, [pmIm]Br and its applications.

4. General principles of qualitative analysis:

Principle of flame testing ï theory of testing acid radicals (simple and interfering). Principle of grouping of cations ï theory of testing cations.

5. Inorganic analysis by using green methods:

1. Analysis of simple acid radicals: carbonate, sulfide, sulfate, thiosulfite, chloride, bromide, iodide, nitrate.
2. Analysis of interfering acid radicals: fluoride, oxalate, borate, phosphate, arsenate, arsenite.
3. Elimination of interfering acid radicals and identifying the groups of basic radicals.
4. Analysis of basic radicals (group-wise): Lead, copper, bismuth, cadmium, tin, antimony, iron, aluminium, arsenic, zinc, manganese, nickel, cobalt, calcium, strontium, barium, magnesium, ammonium.
5. Repeating the tests in no. 04
6. Repeating the tests in no. 04
7. Analysis of a mixture-I containing three cations and three anions (of which one is interfering type).
8. Analysis of a mixture-II containing three cations and three anions (of which one is interfering type).
9. Analysis of a mixture-III containing three cations and three anions (of which one is interfering type).
10. Analysis of a mixture-IV containing three cations and three anions (of which one is interfering type).

Note: 1. The students must have exposure of at least two analytical instruments.

2. Four experiments must be performed from section 2 & 5.

Suggested Books:

1. H. Denny, W. Roesky, Chemical Curiosites, WILEY VCH, 1996.
2. G. Marr and B. W. Rocket, Practical inorganic chemistry, University Science Books, 1999.
3. G. Pass and H. Sutcliffe, Chapman and Hall, Practical Inorganic Chemistry, London, 2nd edition, 1974.
4. J. Mendham, R. C. Denney, J. D. Barnes, M Thomas, Vogelôs Textbook of Quantitative Analysis, Pearson education, 5th edition, 2006.
5. G. Svehla, Vogelôs Textbook of Quantitative Analysis, Pearson education, 2006.

6. Anil J. Elias, A Collection of interesting General Chemistry Experiments, Orient Longman Limited, Universities Press (India) Pvt. Ltd., 2008.
7. http://dst.gov.in/green-chem.pdf

MSCH-21106 Organic Chemistry Lab-I

External Marks: 100 **L T P**
Internal marks: 50 **0 0 6**
Total Marks: 150

1. Qualitative Organic Analysis

Separation and purification of components of binary mixture (Solid/solid, solid/liquid and liquid/liquid) on the basis of solubility behaviour and solvent extraction, and their identification and conformation by chemical tests and preparation of suitable derivative. Preparative TLC separation for IR and PMR spectral studies of the respective component.

2. Organic Synthesis

Benzoylation : Hippuric acid
Oxidation : Adipic acid/p-Nitrobenzoic acid
Aldol condensation : Dibenzalacetone/Cinnamic acid
Sandmeyer's reaction : p-Chlorotoluene
Benzfused Heterocycles : Benzimidazole
Cannizzaro's reaction : p-Chlorobenzaldehyde as substrate
Friedel Crafts reaction : S-Benzoylpropionic acid
Aromatic electrophilic substitution : p-Nitroaniline / p-Iodoaniline
The products may be characterized by spectral techniques.

Suggested Books:

1. Vogels's Textbook of Practical Organic Chemistry, 5th Edition ELBS (Longman), 1996.
2. F.G. Mann and B.C. Saunders, Practical Organic Chemistry, 5th Edition, Orient Longman Limited, 1986.

MSCH-21201 Organic Chemistry-II

External Marks: 100 **L T P**
Internal marks: 50 **4 1 0**
Total Marks: 150

Course Objective:

1. To understand principles of stereochemistry.
2. To understand structures of supramolecular chemistry.
3. To understand applications of photochemistry.

1. Principles of Stereochemistry

Configurational and conformational isomerism in acyclic and cyclic compounds, stereogenicity, stereoselectivity, enantioselectivity and diastereoselectivity. Configurational and conformational effects on reactivity and selectivity/specificity. Elements of symmetry, chirality, molecules with more than one chiral centres, chirality of organic molecules without chiral centres (biphenyls, allenes, spiranes) and due to helical shape. Enantiotopic and diastereotopic atoms, groups and faces. Stereoselective and stereospecific synthesis.(11)

2. Supramolecular Chemistry

Nature of supramolecular interactions, pre- organization and complementarity. Classification of supramolecular host-guest compounds- crown ethers, calixarenes, cyclophanes, cryptands, cyclodextrins, fullerenes, micelles and vesicles. Supramolecular reactivity and catalysis, supramolecular photochemistry, molecular machines based on catenanes and rotaxanes. (11)

3. Photochemistry: Basic principles of photochemistry, photochemistry of alkenes, carbonyl compounds, arenes and fullerenes, photooxidation and photoreduction, Organic solid state photochemistry, chemiluminescent reactions, Barton reaction, di-p-methane rearrangement. Principles and applications of photochemical reactions in organic chemistry, pericyclic reactions-electrocyclization, cycloaddition, sigmatropic rearrangements and related concerted reactions. Applications of pericyclic reactions in synthesis. (11)

4. Metal Salt Catalysis

Fundamental reaction steps of transition metal catalysed reaction, oxidative-addition reactions, elimination reactions, cleavage of C-H bonds, migration reaction and insertion reaction. Homo/heterogeneous catalysis by transition metal complexes. Hydrogenation reaction, alkene isomerisation, hydrosilylation and hydroboration reaction, alkene hydrogenation, reaction of CO and hydrogen, hydroformylation of unsaturated compounds,

carbonylation reactions, C-C cross coupling and related reactions, reactions of conjugated dienes, reactions of alkynes, alkene and alkyne metathesis, phase transfer catalysis, C-H activation using metal salts, Suzuki reaction, Heck reaction, Negishi coupling, Stille reaction, Sonogashira coupling reactions. (12)

Suggested Books:

1. B. Smith, Jerry March, March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 6th Edition, Wiley-Interscience, 2007.
2. Carey F.R., Sunberg R.J., Advanced Organic Chemistry, 5th edition, Springer, 2007.
3. J.W Steed and J.L. Atwood, Supramolecular Chemistry, John Wiley & Sons, NY, 2000.
4. E.L. Eliel, S.H. Wilen, Stereochemistry of Organic Compounds, Wiley, 1994.
5. P.S. Kalsi, Stereochemistry: Conformation and Mechanism, New Age International Edition, 7th Edition, 2009.
6. N.J. Turro, V. Ramamurthy and J.C. Scaiano, Principles of Molecular Photochemistry, An Introduction, University Science Books, 2008.
7. W.M. Horspool and P.S.Song (Ed.), Handbook of Organic Photochemistry and Photobiology, CRC Press, 1995.

MSCH-21202 Symmetry and Group Theory

External Marks: 100 **L T P**
Internal marks: 50 **4 1 0**
Total Marks: 150

Course Objective:

1. To educate students about the importance of symmetry elements and operations.
2. To acquaint students with character tables.
3. To develop an understanding of molecular orbital theory and ligand field theory with respect to symmetry properties.

1. Symmetry elements and operations

Symmetry planes and reflections, inversion centre, proper axes and proper rotations, improper axes and improper rotations. (05)

2. Relations among Symmetry Elements

Products of symmetry operations, equivalent symmetry elements and equivalent atoms, general relations among symmetry elements and operations, symmetry point groups, symmetry classification of molecules, virtual labs. (08)

3. Representations of groups: Important rules about irreducible representations and their characters, relationship between reducible and irreducible representations with examples. Construction of character tables. (08)

4. Molecular orbital theory and its applications: Symmetry based selection rules for cyclization reactions, dimerization of ethylene, Diels-Alder reactions. (06)

5. Molecular orbital theory for inorganic compounds: Transformation properties of atomic orbitals, molecular orbitals for sigma bonding in tetrahedral and octahedral molecules. (10)

6. Ligand field theory: Introduction, Electronic structure of free atoms and ions, splitting of levels and terms in a chemical environment, construction of energy level diagram. (08)

Suggested Books:

1. F. A. Cotton, Chemical Applications of Group Theory, Wiley, 3rd edition, 2004.
2. J.N. Murrell, S.F.A. Kettle, John M Tedder, Valence Theory, John Wiley, 1970.
3. R. B. Woodward and R. Hoffmann, Conservation of Orbital Symmetry, Academic Press, 1970.

4. B .N. Figgis, Introduction to Ligand Fields, John Wiley, 1996.
5. Salahuddin Kunju & G. Krishnan, Group Theory and Its Applications in Chemistry, PHI Learning Private Limited, New Delhi, 2010.
6. http://vlab.co.in/ba_labs_all.php?id=9.

MSCH-21203 Spectroscopy- I

External Marks: 100 **L T P**
Internal marks: 50 **4 1 0**
Total Marks: 150

Course Objective:

1. To educate students about molecular absorption and emission spectroscopy.
2. To understand how the interaction of electromagnetic waves with the matter leads to wonderful results.
3. To educate students about atomic absorption and emission spectroscopy.

1. Introduction

Characterization of electromagnetic radiation, the quantization of energy. Regions of the spectrum, representation of the spectrum. Basic elements of practical spectroscopy, Fourier transformation spectroscopy, computer averaging, stimulated emission. (6)

2. Microwave Spectroscopy

The rotation of the molecules, rotational spectra, diatomic molecules, polyatomic molecules, techniques and instrumentation, chemical analysis by microwave spectroscopy. Microwave oven. (7)

3. Infra-red and Raman Spectroscopy

Introduction, the vibrating diatomic molecule, the diatomic vibrating rotator. The vibration-rotation spectrum of carbon monoxide. Breakdown of the Born-Oppenheimer approximation: The interaction of rotations and vibrations. The vibrations of polyatomic molecules and influence of rotation on the spectra of polyatomic molecules. Analysis by infrared techniques ï identity by finger printing and functional groups, techniques and instrumentation.

Pure rotational Raman spectra, vibrational Raman spectra. Polarization of light and the Raman effect, Structure Determination from Raman and infrared spectroscopy, techniques and instrumentation, near infrared FT-Raman spectroscopy. Comparison of infrared and Raman spectra. (10)

4. Electronic Spectroscopy

Principles of absorption spectroscopy, chromophore concept, solvent effects, Woodward-Fischer rules. Applications of electronic spectroscopy. Stereochemical factors. Absorption spectra for charge-transfer complexes, Electronic absorption spectroscopy for chemical analysis. (10)

5. Atomic Absorption and Emission Spectroscopy

Introduction, elementary theory, instrumentation. Graphite furnace and cold vapour technique, interferences, background correction methods, Applications of AAS. Emission spectra, flame emission spectroscopy, evaluation methods, plasma emission spectroscopy ICP instrumentation. Applications of flame photometry. (9)

6. Luminescence Spectroscopy: Principles of luminescence spectroscopy, applications for inorganic & organic compounds. (3)

Suggested Books:

1. C. N. Banewell, Fundamentals of Molecular Spectroscopy, 4th Edition, Tata Mc Graw-Hill Publication, 1994.
2. G. N. Barrow, Introduction to Molecular Spectroscopy, International Mc.Grw Hill Edition, 4th edition, 1993, UNIT II.
3. D. H. Williams and I. Flemings, Spectroscopic Methods in Organic Chemistry, Tata Mc Graw-Hill Publication, 6th edition, 2007.
4. Drago R.S., Physical Methods in Chemistry, 3rd ed, Philadelphia, London, W.B.
5. Saunders Company, 1992.
6. W. Kemp, Organic Spectroscopy, ELBS Mcmillan, 3rd edition, 1991.

MSCH-21204 Quantum Chemistry

External Marks: 100 **L T P**
Internal marks: 50 **4 1 0**
Total Marks: 150

Course Objective:

1. To learn basic mathematical concepts in quantum chemistry.
2. To understand valence-bond and molecular orbital approaches.
3. To understand and apply perturbation theory.

1. Preparation/revision of basic mathematical concepts

Vectors, dot, cross and triple products etc, gradient, divergence and curl. Matrices ï addition, multiplication, adjoint and transpose, special matrices (symmetric, skew-symmetric, hermitian, skew-hermitian, unit, diagonal, unitary etc.). Linear equations, eigen value problem, diagonalization, determinants. Calculus and elementary differential equations - all examples be taken from chemistry. Classical mechanics: Introduction, Lagrangeôs and Hamiltonôs equations of motion in classical mechanics, configuration space and phase space. Hermitian operators and their properties. Commutation relations. Postulates of quantum mechanics. Uncertainty principle. Schrodinger wave equation and its interpretation. (11)

2. Linear harmonic oscillator

Linear harmonic oscillator and its solution in terms of ladder operators (factorization method). Selection rules, expectation values, virial theorem. Hydrogen atom and its complete solution (including solution of the radial equation using factorization method). Spherical harmonics as wave functions of a rigid rotor. Total wave function of the hydrogen like atoms, shapes of atomic orbitals, Radial distribution function. Virial theorem. Angular momentum, spin coupling of angular momenta; spin-orbit coupling. Term symbols from electronic configuration. (12)

3. Approximate methods

Time-Independent (non-degenerate, degenerate states) perturbation theory. Applications of time-dependent perturbation theory. The variation method. LCAO-MO approximation. Comparison of perturbation and variation method. Hartree-Fock equations. configuration interaction. Applications to the electronic structure of many electron atoms, screening, Slater orbitals, Gaussian orbital. (11)

4. The Born-Oppenheimer Approximation

Valence-bond and molecular orbital approaches, their comparison and equivalence limit. Electronic structure of an atomic and polyatomic molecules- an introductory treatment. General molecular orbital theory. The pi-electron approximation. Huckel theory of conjugated systems. Applications to ethylene, butadiene and benzene. (11)

Suggested Books:

1. Atkins P.W. and Friedman R.S., Molecular Quantum Mechanics, 4th edition, Oxford University Press, 2005.
2. McQuarrie D., Quantum Chemistry, 2nd edition, University Science Books, 2007.
3. Levine I.N., Quantum Chemistry, 6th edition, Pubs: Prentice Hall, 2009.
4. Kreyszig E., Advanced Engineering Mathematics, 10th edition, John Wiley, 2012.
5. Ayres F. Jr., Theory and Problems of Matrics, Schaumôs Outline series,McGraw Hill, New Delhi, part 2, 1974.
6. Spiegel M.R., Vector Analysis, Schaumôs Outline Series, McGraw Hill, New Delhi, 1968.
7. Ayres F., Jr. and Mendelson E., Schaum's Outline of Theory and Problems of Differential and Integral Calculus, McGraw hill, New Delhi, 3rd edition, 1990.
8. Pilar F.L., Elementary Quantum Chemistry, 2nd editilon, McGraw Hill, New York, 1990.
9. March N.H., Self-Consistent Fields in Atoms, Pubs: Pergamon Oxford Press, 1975.
10. Chandra A.K., Introductory Quantum Chemistry, Pubs: Tata-McGraw Hill, 4th edition, 2004.
11. Pople J.A. and Beveridge D.L., Approximate Molecular-Orbital Theory, Pubs: McGraw Hill, New York, 1970.
12. Lowe J.P., Peterson, K, Quantum Chemistry, 3rd edition, Academic Press, 2005.

MSCH-21205 Physical Chemistry Lab

External Marks: 100 **L T P**
Internal marks: 50 **0 0 6**
Total Marks: 150

Note: Do any 10 experiments

1) Determine the specific rotation of an optically active compound.
2) Study the kinetics of inversion of cane sugar by polarimetry.
3) Estimate the strength of the strong acid and the weak acid in a mixture by conductometric titration.
4) Determine the rate constant of saponification of methyl acetate conductometrically at room temperature.
5) Determine the ionization constant (K_a) of a weak acid by conductometric method at room temperature and find the equivalent conductance at infinite dilution (λ_∞) of a weak acid by graphical extrapolation (Verification of Ostwaldôs dilution law).
6) Potentiometrically estimate the strength of Mohrôs salt with the help of a standard potassium dichromate solution. Find the E_0, Fe^{3+} / Fe^{2+} using graphical methods.
7) Potentiometrically estimate the strength of AgNO3 solution with a standard KCl solution. Determine the solubility product (K_{sp}) of AgCl at room temperature.
8) Estimate the strength of a weak acid (monobasic/dibasic) pH-metrically. Find pK_a of this acid at room temperature using a graphical procedure.
9) Study the kinetics of the reaction ($KI + K_2S_2O_8$) by colorimetric method and determine the rate constant of the reaction at room temperature.
10) Test the validity of Lambert-Beerôs law for $KMnO_4$ solution. Construct similarly the calibration curve for $K_2Cr_2O_7$ solution and hence determine the concentration of an unknown $K_2Cr_2O_7$ solution.
11) Study the kinetics of iodination of acetone in presence of acid. Hence find out the order with respect to iodine/acetone/acid.
12) Determine the critical solution temperature of phenol-water system.
13) Determine the solubility product (Ksp) of PbI_2 and verification of Debye-Hückel limiting law.
14) Determination of E_0 of quinhydrone electrode.

Suggested Books:

1. Berry, Rice and Ross, Physical Chemistry (Topics in Physical Chemistry), 2nd edition, Oxford University Press, 2000.
2. Moore, Physical Chemistry, 5th edition, prentice hall, 1999. 3. Atkins, Physical Chemistry, 9th edition, W.H. Freeman & Co., 2010.

3. Levine, Physical Chemistry, 6th edition, McGraw-Hill, 2002.
4. K.J. Laidler, Chemical Kinetics, 3rd edition, Pearson Education India, 1987.
5. Zemansky and Dittman, Kinetics and Mechanism;
6. Zemansky and Dittman, Heat and Thermodynamics, 7th edition, McGrawHill, 2006.
7. Saha and Srivastava, A Treatise on Heat, 3rd edition, The Indian Press, 1950.
8. Glasstone, An Introduction to Electrochemistry, Affiliated East West Press Private, Limited, 1974.
9. Bockris and Reddy, Modern Electrochemistry 2A & 2B, Springer, 2000.

MSCH-21206 Organic Chemistry Lab-II

External Marks: 100 **L T P**
Internal marks: 50 **0 0 6**
Total Marks: 150

1. Beckman Rearrangement
I. Benzene-Benzophenone Benzophenone Oxime Benzanilide
II. Benzene Acetophenone Acetophenone Oxime-Acetanilide.
III. Cyclohexanone Oxime-Caprolactam

2. Benzillic acid Rearrangement I. Benzoin-Benzil-Benzillic-acid
II. Benzoin-Benzil-Benzil monohydrazone

3. Fischer Indole Synthesis
I.N-Arylmaleinilic acid N-aryl maleimide
II. 1, 2, 3, 4- Tetrahydrocarbazole
III. 2-Phenylindole from Phenylhydrazone

Suggested Books:
1. Vogelôs Text Book of Practical Organic Chemistry, 5th edition, Prentice Hall, 1996.
2. Julius B. Cohen, Practical Organic Chemistry, 1910.

MSCH-21301 Inorganic Chemistry-II

External Marks: 100 **L T P**
Internal marks: 50 **4 1 0**
Total Marks: 150

Course Objective:

1. To fully understand the chemistry of transition and inner transition elements.
2. To acquaint with organometallic chemistry**.**
3. To know the structures of ionic solids.
4. To know the advancement of inorganic chemistry in medicine and inorganic compounds in material science.

1. Survey of Transition Metal Chemistry

Electronic configuration, general characteristics, oxidation states, pi-acid ligands, metal complexes, metal- metal bond, quadruple bonds. Transition metal catalyzed reactions**:** Oxidative addition, Elimination reactions and migration reactions. Mechanism of inorganic reactions: Inner sphere, outer sphere, trans effect. (8)

2. Coordination Chemistry

Coordination number and structures of coordination complexes. Theory of bonding- crystal field and molecule orbital theory. JT distortion, electronic spectra of coordination compounds. Tanabe-Sugano diagrams, stereochemistry of non-rigid and fluxional molecules. Thermodynamic aspects of coordination complexes: lrving William Series. Kinetic aspects: reactions and aquation rates, electron transfer reactions. Reaction mechanisms of inorganic reactions. Redox reactions. (10)

3. Chemistry of Inner Transition Elements

Electronic configuration, oxidation states, coordination numbers and stereochemistry, Magnetism and spectra, complexes and organometallic chemistry of lanthanides and actinides**.** (7)

4. Organometallic Chemistry

Structure, bonding and reactivity studies of metal carbonyls, nitrosyls, dinitrogen complexes, metal alkyls, carbenes, carbines and carbides. Metallocenes and related chemistry. Homogeneous and heterogeneous catalysis. Organometallic complexes with metal-metal bonds. (10)

5. Inorganic Compounds in Medicine and Materials

Metal complexes in organic reactions, cis-platin, gold complexes, technetium complexes, metal nano-particles in heterogeneous catalysis, metal embedded polymers as functional materials, metal complexes in display technologies. Inorganic vapochromic materials, molecule-based magnetic materials. DNA cleavage by transition metal complexes, anti-cancer drugs, therapeutic drugs, metal and non-metals in PET. (10)

Suggested Books:

1. D. F. Shriver and P. W. Atkins, Inorganic Chemistry, 4th edition, Oxford University, Oxford, 2006.
2. B. N. Figgis, Ligand Field Theory, Wiley Eastern,1976.
3. F. A .Cotton and G .Wilkinson et a, Advanced Inorganic Chemistry, 6th edition, John Wiley & Sons, 2003.
4. J. E. Huheey et al, Inorganic Chemistry, 4th edition, Pearson, 2005.
5. B. Douglas et. al, Concepts & Model of Inorganic Chemistry, John Wiley & Sons, New York, 3rd edition, 1994.
6. N. N. Greenwood, Chemistry of Elements, Pergamon Press, 2000.

MSCH-21302 Spectroscopy-II

External Marks: 100 **L T P**
Internal marks: 50 **4 1 0**
Total Marks: 150

Course Objective:

1. To provide students knowledge of various resonance and ionization techniques.
2. To educate the students about the elucidation of structures based on these techniques.
3. To make them familiar with some advanced NMR techniques.

1. Nuclear Magnetic Resonance Spectroscopy

1H-NMR spectroscopy: Introduction, chemical shift, shielding and equivalence, nuclear magnetic resonance spectrometer, spin- spin splitting rule, coupling constant, protons on oxygen, nitrogen and sulphur. Quadrupole broadening and decoupling. The effect of solvent on chemical shift, chemical shift reagent, chiral resolving agents. Determining absolute and relative configurations via NMR, nuclear overhauser effect difference spectra.

13C NMR spectroscopy: Introduction, proton-coupled and decoupled 13C spectra, spin-spin splitting of carbon-13 signals, NOE, molecular relaxation process, DEPT, equivalent carbons, compounds with aromatic ring, carbon-13 NMR solvents, hetero-coupling , coupling constant , magnetic equivalence, first-order and second order spectra, coupling in heteroaromatic system.

Advanced NMR techniques: Pulse Sequences and Field Gradients, DEPT experiment, two dimensional spectroscopic methods, correlation spectrometry, COSY, HETCOR, inverse detection method, NOESY experiment, magnetic resonance imaging. Solving a structural problem using combined 1-D and 2-D techniques. (15)

2. Nuclear Quadruple Resonance Spectroscopy

Introduction, experimental considerations, fundamentals of NQR spectroscopy, origin of EFG. Measurement of energy differences between two spin states, the asymmetry parameter, effects of magnetic field. Interpretation of the spectra, applications of technique to halogen compounds, transition metals. Complications in spectra. (7)

3. Electron Paramagnetic Resonance Spectroscopy:

Introduction, principle, presentation of spectrum, hyperfine splitting in isotropic systems involving ore than one nucleus, esr spectrum of benzene radical anion, methyl radical, CH2OH, cyclopentadienyl radical, cyclopentatrienyl radical, pyrazine anion with 23Na and 30K counter ion, nitrosyl nitroxide. Factors affecting magnitude of g values, zero field

splitting and Krammerôs degeneracy. Qualitative survey of EPR spectra of first row transition metal ion (, d2, d3, low spin d5, d5, high spin d6, d7, d9 system. (7)

4. Mossbauer Spectroscopy

Principles of Mossbauer spectroscopy, experimental considerations, the spectrum and its parameters. Simple spin states, higher spin states, chemical shift, quadrupole effects. Effects of a magnetic field, applications of Mossbauer spectroscopy ï interpretation of Mossbauer spectra. (7)

5. Mass Spectrometry

Overview of the mass spectrometer, Ionization methods, mass analysis, Determination of molecular weight and formulae. Structural analysis and fragmentation patterns, strategic approach. Computerized matching of spectra with spectral libraries. (9)

Suggested Books:

1. R. M. Silverstein and F. X. Webster, Spectroscopic Identification of Organic Compounds, 6th Ed., John Wiley & Sons, New York, 1998.
2. D.L. Pavia, G. M. Lampman, George S. Kriz, James R. Vyvyan, Introduction to Spectroscopy, 4th Ed., Brooks India, 2008.
3. C. N. Banewell, Fundamental of Molecular Spectroscopy, 4th Edition, Tata Mc Graw-Hill Publication, 1995.
4. G. N. Barrow, Introduction to Molecular Spectroscopy, Mc Graw Hill Publications, 1980.
5. D. H. Williams and I. Flemings, Spectroscopic Methods in Organic Chemistry, Tata Mc Graw-Hill Publication, 1994.
6. R. S. Drago, Physical methods in Inorganic Chemistry, Reinhold Publishing Corporation, 1965.

MSCH-21303 Computational Skills and Simulations in Chemistry

External Marks: 100 **L T P**
Internal marks: 50 **4 1 0**
Total Marks: 150

Course Objective:

1. To gain the basic understanding of computer and computer language.
2. To understand various methods of numerical solutions of differential equations.
3. To gain the knowledge of application of regression analysis to probability distribution.

1. C/C++ Programming

Introduction to algorithm, Flow charts, Problem solving methods, Need of programming languages. C character set, Identifiers and keywords, Data types, Declarations, Statement and symbolic constants, Input-output statements, Pre-processor commands, Operators, expressions and library functions, Control statements: Conditional, Unconditional, Bi-directional, Multi-directional and loop control structures, Functions, Arrays, Strings, Introduction to Pointers, Structure and union, Files. (12)

2. System of Linear Equations

Gauss- elimination method, Croutôs method, inverse of a matrix. Iterative methods: Jacobiôs method, Gauss-Seidel Method. Numerical differentiation and integration - Newton-Cotes formulae. (10)

3. Numerical Solutions of Differential Equations

Picardôs Method, Taylorôs series Method, Eulerôs Method, Modified Eulerôs method, Runge-Kutta Methods. Numerical solution of partial differential equations: finite difference methods. (13)

4. Statistics

Correlation analysis and regression analysis, Probability-addition and multiplication theorems. Probability distributions: Binomial, Poisson and normal distribution. (10)

Suggested Books:

1. R.Singh, I.Singh, Expert C++ Programming, Khanna Book Publishing Co. (P) Ltd.
2. Kerninghan B.W. and Ritchie D.M., The C programming language, PHI (1989)
3. Kanetkar Yashawant, Let us C, BPB (2007).
4. Rajaraman V., Fundamentals of Computers, PHI (2004).
5. S.S. Sastry, Introductory Methods of Numerical Analysis, PHI Learning Pvt. Ltd., 4th edition, 2005.

6. Conte and de Boor, Elementary Numerical Analysis, McGraw Hill, New York, 1990.
7. John H. Mathews, Numerical Methods for Mathematics, Science and Engineering, 2nd Edn., Prentice Hall, New Delhi, 2000.
8. Gupta and Kapoor, Fundamentals of Mathematical Statistics, Sultan Chand & Sons, 2012.
9. Goon, Gupta and Das Gupta, Fundamentals of Statistics, World Press Private, 2005.
10. Mckean, J.W. and Craig, A.T. Mukhopadhyay, P, Mathematical Statistics.

MSCH-21304 Polymers

External Marks: 100 **L T P**
Internal marks: 50 **4 1 0**
Total Marks: 150

Course Objective:

1. To understand various terms related to polymers.
2. To learn various types of polymer mechanisms and their kinetics.
3. To learn how to characterize polymer structures.

1. Introduction to Polymers

Polymer terminology-fatigue, tensile strength, impact strength, breaking load, crimp, denier, elongation at break, filament, yarn, filament yarn, porosity, resilience, staple fibre, bursting strength, tex, creep, tenacity. IUPAC nomenclature of vinyl, nonvinyl polymers, copolymers and end groups. Abbreviations for polymers. Introduction to industrial polymers-plastics (commonly used commodity- & engineering plastics, thermoplastic- & thermosetting plastics), fibres (commonly used natural & synthetic fibres), elastomers (commonly used natural & synthetic rubbers), coatings and adhesives. Comparison of properties of various types of polymers. Polymer recycling. (6)

2. Polymerization Mechanisms

Mechanism of free radical chain polymerization & ionic chain polymerization-initiators, inhibitors & stereochemistry. Mechanism of coordination chain polymerization (Ziegler-Natta, Cossee), polycondensation step polymerization, polyaddition step polymerization & ring opening step polymerization. (6)

3. Kinetics of Polymerization Mechanisms

Kinetics of free radical chain polymerization, ionic chain polymerization, catalysed and non catalysed polycondensation polymerization including kinetic chain length, chain transfer reactions. (5)

4. Average Molecular Weight of Polymers

Number average molecular weight ï its measurement by osmometry (membrane & vapour phase), end group analysis, mass spectrometry. Weight average molecular weight ï its measurement by light scattering method (dissymmetry method & Zimm plot method). Viscosity average molecular weight ï its measurement by viscometry. Determination of molecular weight distribution by gel permeation chromatography (size exclusion chromatography). (6)

5. Chemical Structure & Polymer Morphology

Macrostructure of polymers**.** Geometrical isomerism & optical isomerism, Tacticity, degree of crystallinity, liquid crystallinity, crystallizability, crystallites (bundles), spherulites, polymer single (ideal) crystals. Glass transition temperature- concept of glassy state, viscoelastic state, viscofluid state for amorphous and crystalline substances including polymers. Specific volume change vs temperature curves. (5)

6. Polymer Properties

Mechanical properties - tensile strength, compressive strength, flexural strength, impact strength, toughness, fatigue, yield point, elongation at break, tensile modulus, relaxation & retardation (creep) phenomena. Thermal stability, flammability & flame resistance, chemical resistance, degradability, electrical conductivity, nonlinear optical properties. Polymer additives to modify mechanical, surface, chemical, aesthetic & processing properties. (6)

7. Fibres Reinforced Polymer Composites

Introduction to composites. Polymer matrix materials & fibres reinforcement. Types of fibres- glass, metal, graphite, boron, alumina, silicon carbide, aramid, quartz & silica fibres. Advantages & disadvantages of polymer composites. (5)

8. Characterization Techniques of Polymers

Infrared, Raman, NMR, ESR, UV-Vis, fluorescence studies. X-ray scattering, SEM, thermal-DSC, DTA, TMA, TGA studies. (6)

Suggested Books:

1. D. Campbell and J.R. White, Polymer Characterization: physical Techniques, Chapman and Hall, New York, 1989.
2. Malcolm P. Stevens, Polymer Chemistry an Introduction, Oxford University Press, 3rd edn, Indian Edition, reprint, 2011.
3. A.H. Fawcett, Polymer Spectroscopy, Wiley, New York, 1996.
4. R.J. Young, Spectroscopy of Polymers, Wiley, New York, 1996.
5. M. Lewin, S.M. Atlas, E.M. Pearce, Flame Retardant Polymeric Materials, Plenum Press, New York, 1975.
6. E.M. Pearce, Y.P. Khanna, D. Raucher, Thermal Characterization of Polymeric Materials, Academic Press, New York, 1981.
7. I.M. Ward, Mechanical Properties of Polymers, Wiley Interscience, New York, 1971.
8. Jan M. Gooch, Encyclopedic Dictionary of Polymers, Springer, 2007.
9. Anita J. Brandolini, Deborah D. Hills, NMR Spectra of Polymers & Polymer Additives, Marcel Dekker, New York, 2000.

10. Fred W. Wilmeyer, Text book of Polymer Science, A. Wiley Intersciense Publication, 1994.
11. V. R. Gowariker, V. R. Gowariker, N.V. Viswanathan, J. Sreedhar; Polymer Science, New Age International, 1986.

MSCH-21305 Computational Skills and Simulations in Chemistry Lab

External Marks: 100 **L T P**
Internal marks: 50 **0 0 6**
Total Marks: 150

A. Programming in C++ language (Do any eight)

1. Calculation of mean, median, mode.
2. Solution of a quardratic equation.
3. Calculation of Bohr orbit from de Broglie Lambda for electron.
4. Calculation of wave number and frequency from value of wavelength.
5. Calculation of van der Waals radii.
6. Calculation of linear regression.
7. Rate constant of a 1^{st} order reaction, 2^{nd} order reaction.
8. Calculation of lattice energy using Born Lande equation.
9. Addition, multiplication and solution of inverse of 3 X 3 matrix.
10. Calculation of average molecular weight of a polymer containing n1 molecules of molecular weight m1, n2 molecules of molecular weight M2 and so on
11. Program for calculation of molecular weight of organic compound containing C, H, N, O and S.
12. Calculation of reduced mass of diatomic molecule.
13. Calculate the RMS and most probable velocity of a gas.
14. Calculate the ionic mobility from ionic conductance values.

B. Introduction to Web and Internet

LAN and E-mail, Importance of Internet; Types of search engines: Basic components of browsing page; importance of networks; networking personal computers; importance of E-mailing, search engines in chemical sciences.

C. Chemdraw/Chemwind

Drawing and editing molecular structures using Chemwind and Chemdraw templates, Sigma Plot and Sigma Statistical tool handling.

D. Softwares

To familiarize with different software packages such as ORIGIN for plotting, MOLDEN for model building, GAMESS Gaussian for quantum chemical calculations, MOLECULAR DOCKING to predict the binding affinity between two molecules, SAR (structureï activity relationship) to study the relationship between a drug's molecular structure and the drug's biological activity.

Suggested Books:

1. K.V. Raman, Computers in Chemistry, Tata McGraw Hill.
2. Mullish Cooper, The spirit of C, An Introduction to Modern Programming.
3. Sudhir K.Bansal, Anshu Bansal, Computers for Chemists, Pragati Prakashan.
4. R.Singh, I.Singh, Expert C++ Programming, Khanna Book Publishing Co.
F. Jensen, Introduction to Computational Chemistry, John Wiley & Sons, 1998.
5. Warren J. Hehre, A Guide to Molecular Mechanics and Quantum Chemical Calculations, 2003.
6. Christopher Cramer, Essentials of Computational Chemistry, Theories & Models, 2nd edition, Wiley, 2002.

MSCH-21306 Inorganic Lab-II

External Marks: 100 **L T P**
Internal marks: 50 **0 0 6**
Total Marks: 150

Course Objective:

1. To know the significant figures and various errors and to understand the principle of working of balances.
2. To become aware of handling of glass wares used in titrimetry.
3. To know the principles of various types of titrimetric analysis.
4. To learn the theory and importance of analytical chemistry.
5. To know the safe working in the Lab and Lab hygiene.
6. To know the methods of analyzing the chemicals by applying the electroanalytical techniques.

1. Introduction to Quantitative Analysis

Introduction ï types of quantitative analysisï theory of significant figures ï error analysis ï principles of chemical balances (double-pan and single-pan) ï apparatus used in titrimetric analysis ï handling of chemical balances and other apparatus ï concept of molecular weight, formula weight, equivalent weight ï concentrations of solutions ï molarity, formality, normality and weight percentage.

2. General Principles of Titrimetry

Principle of titrimetry ï primary and secondary standards ï preparing standard solutions ï standardising the secondary standard solutions ï types of titrimetric analyses ï principal reactions ï concepts of acids, bases, oxidants, reductants ï theory of indicators ï calculations for strengths of solutions and the amounts of substances in solutions.

3. Laboratory Hygiene and Safety

Storage and handling of corrosive, flammable, explosive, toxic, carcinogenic and poisonous chemicals. Simple first aid procedures for accidents involving acids, alkalies, bromine, burns and cut by glass. Threshold vapour concentration - safe limits. Waste disposal.

4. Complexometric Titrations

Determination of calcium in the presence of magnesium using EGTA as titrant. Determination of the total hardness (permanent and temporary) of water. Determination of calcium in the presence of barium using CDTA as titrant.

5. Redox Titration

(a) Determination of chlorate, preparation of 0.1M cerium(IV) sulphate solution.
(b) Determination of copper, determination of dissolved oxygen.
(c) Determination of hydrogen sulphide.
(d) Determination of antimony & arsenic.

6. Electroanalytical Techniques- pH metric, conductometric and amperometric titration

Representative acid-base and redox titrations.

7. Colorimetry and Spectrophotometry

(a) Determination of max the absorption curve and concentration of a substance.
(b) Simultaneous spectrophotometric determination (chromium and manganese).
(c) Spectrophotometric determination of pK value of an indicator.
(d) Determination of copper(II) with EDTA
(e) Determination of iron(III) with EDTA.

8. Atomic Absorption Spectroscopy

(a) Determination of cations by AAS
(b) Determination of magnesium and calcium in tap water
(c) Determination of trace elements in contaminated soil
(d) Determination of vanadium in lubricating oil, determination of trace lead in a ferrous alloy.

Suggested Books:

1. J. Mendham, R.C. Denney, J.D. Barnes, and M. Thomas, Vogelôs Textbook of Quantitative Analysis, 6th Ed., Pearson Education, 2000, 3rd reprint.
2. R. Gopalan, P.S. Subramaniam and K. Rengarajan, Elements of Analytical Chemistry, 3rd edition, Sultan Chand and Sons, New Delhi, 2003.

MSCH-21401 Photochemistry

External Marks: 100 **L T P**
Internal marks: 50 **4 1 0**
Total Marks: 150

Course Objective:

1. To understand various types of photo reactions.
2. To learn photochemical reactions in inorganic chemistry.
3. To study kinetics of photochemical reactions.

1. Organic Photochemistry

Organic photochemistry: Photochemical reactions, fate of excited molecules, Jablonski diagram, Norish type I and Norish II reactions, photoreduction (of ketones), photoaddition reactions, Paterno-Buchi reactions, di-pi methane rearrangement, photo oxidation (formation of peroxy compounds), photo-iIsomerization (cis-trans isomerisation), photo-addition of olefin and amines to aromatic compounds, photo-rearrangements; Photo-Fries rearrangement. (12)

2. Inorganic Photochemistry

Photo-substitution, -redox, -isomerization, and - rearrangement reactions in inorganic complexes, photovoltaic and photo-galvanic cells- photo-electrochemical cells- photo assisted electrolysis of water, application of metal complexes in solar energy conversions. (10)

3. Physical Photochemistry

Absorption and emission of radiation-Frank Condon principle, spin allowed and spin forbidden transitions. Radiative processes- fluorescence and phosphorescence (factors affecting fluorescence and phosphorescence and theory) prompt and delayed fluorescence and quenching of fluorencence- static and dynamic quenching-Stern Volmer equation, Non-radiative processes, theory of radiationless transition, internal conversion and intersystem crossing. (12)

4. Technique and Applications of Photochemistry

Techniques and applications of photochemistry ï quantum yields- experimental determination of quantum yield, actinometry-chemical actinometry, steady state treatment of quantum yield- reasons for low and high quantum yield- life time measurement- relative and non-relative lifetime measurement- kinetics of photochemical reactions, photosenstized reactions. (10)

Suggested Books:

1. Principles of Molecular Photochemistry: An Introduction.
2. Nicholas J. Turro, Modern Molecular Photochemistry.

MSCH-21402 Environmental Chemistry

External Marks: 100 **L T P**
Internal marks: 50 **4 1 0**
Total Marks: 150

Course Objective:

1. To understand how to analyse various constituents of water.
2. To have detailed study of air pollutants.
3. To have knowledge of toxicology of various organic compounds.

1. Commonly used terms, environmental segments, **n**atural cycles of environment, environmental chemistry of water, water pollution, water treatment operations, advanced waste water treatment. (10)

2. Analysis of major constituents in water, analysis of common ions at low concentration in water, analysis of trace pollutants in water. (10)

3. The atmosphere and atmospheric chemistry, air pollutants, organic air pollutants, atmospheric analysis of gases, atmospheric analysis of particulates, soil formation, soil properties, analysis of soil sediments and biological specifications. (12)

4. Toxicological chemistry, toxicology of some organic compounds, reactions and rate of hazardous wastes, hazardous waste reduction and minimization and physical methods of treatment of hazardous waste, chemical methods of treatment of hazardous waste. (13)

Suggested Books:

1. De., A.K., Environmental Chemistry, 5th Ed., New Age International (P) Limited, New Delhi, 2003.
2. Fifield F.W. and P.J. Hains, Environmental Analytical Chemistry, Blackie Academic and professional , Glasgow, UK, 1995.
3. Gary, W. Vanloon. Stephen J. Duffy, Environmental Chemistry, A global Prospective, Oxford University Press, 2010.
4. John P. Hager, Barry J Hansen, John F. Pusateri, William P. Imrie, V. Ramachandran, Extraction and Processing for Treatment and Minimization of Waste, the Mineral, Metal and Material Society, Pannsylvania, 1994.
5. Rao. C.S., Environmental Pollution Control Engineering, New Age International, New Delhi, 2007.

MSCH-21403 Analytical Principles and Instrumental Method of Analysis

External Marks: 100 **L T P**
Internal marks: 50 **4 1 0**
Total Marks: 150

Course Objective:

1. To learn the theory and importance of analytical chemistry.
2. To acquire knowledge about various methods of quantitative estimations.
3. To know the methods of analyzing the chemicals applying the electroanalytical and thermogravimetric instruments.
4. To know the methods of separating the mixture of compounds by chromatographic techniques.
5. To get familiar with various microscopic and diffraction methods of analysis.

1. Introduction to Analytical Chemistry

Types of analytical methods: Importance of analytical methods in qualitative and quantitative analysis: chemical andinstrumental methods-advantages and limitations of chemical and instrumental methods. Data handling: Introduction, sensitivity and detection limit, noise and sources, Uncertainties, errors, calibrations, mean, standard deviations. Least square fit, computer aided analysis. (5)

2. Thermoanalytical Techniques

Principle of thermo grarvimetry, differential thermal analysis, differential scanning caloimetry - instrumentation for TGA, DTA and DSC-characteristics of TGA and DTA curves - factors affecting TGA and DTA curves. Applications of thermal analysis. (6)

3. Electrochemical Techniques

Basic principle, instrumentation and applications of cyclic voltametry and coulometry, potentiometery, voltametry**, p**olarography. (6)

4. High Performance Liquid chromatography

Principle, instrumentation, supports in HPLC. Applications of HPLC systems, supercritical fluid chromatography (SFC). Recent developments in SFC and applications. (6)

5. Microscopy Techniques

Basic principle, instrumentation and applications of electron microscopy - SEM, TEM, scanning probe microscopy ï AFM. (6)

6. X- Ray Diffraction

Crystal shapes and point groups, reciprocal lattices, unit cells, Miller indices, Braggôs law in reciprocal space, Diffraction pattern assignments, dimensions and contents of the unit cell, X- ray intensities and atomic positions, Fourier synthesis. (6)

7. Neutron Diffraction

Elementary theory of neutron diffraction, study of hydrogen bonds, hydrates and other hydrogen containing compounds, magnetism, limitations. (5)

8. Electron Diffraction

Scattering of electrons by gases, visual method, sector method structure of some molecules studies by electron diffraction, limitation of electron diffraction. (5)

Suggested Books:

1. Douglas A. Skoog and Donald M. West, F.J. Holler, Fundamentals of Analytical Chemistry, 8th edition, Harcourt College Publishers, 2004.
2. Mendham, R. C. Denney, J.D. Barnes, M. Thomas, Vogel's Text Book of Quantitative Chemical Analysis, 6th edition, Pearson Education, 2006.
3. B.K. Sharma, Instrumental Methods of Chemical Analysis, Goel Publishing House, Merrut, 1997.
4. R. Gopalan, P.S. Subramaniam and K. Rengarajan, Elements of Analytical Chemistry, 3rd edition, Sultan Chand and Sons, 2003.
5. S. Usharani, Analytical Chemistry, Macmillan Publishers India, 2000.
6. G. H. Stout and L. H. Jensen, X-ray Structure Determination- A Practical Guide, 2nd edition, Wiley New York, 1989.
7. P.J. Wheatley, Determination of Molecular Structure, Oxford, 1968.
8. D. F. Shriver and P. W. Atkins, Inorganic Chemistry, , 4th edition, Oxford, 2006.
9. Braithwaite and F.J. Smith, Chromatographic Methods, 5th edn., Blackie Academic and Professional, London, 1996.
10. Skoog, Holder, Nieman, Principles of Instrumental Analysis, Fifth edition Thomson Books, 1998.

MSCH-21404 Advanced Chemistry Lab

External Marks: 100 **L T P**
Internal marks: 50 **0 0 6**
Total Marks: 150

Course Objective: The aim and objective of the course on Chemistry Laboratory is to expose the students of M.Sc. to the experimental techniques in general Chemistry, so that they can co-relate the theoretical concepts with the experimental ones and develop confidence to handle sophisticated equipments and prepare reports.

1. **Experimental Methodology**
Students will learn how to design a problem and write hypothesis, set up and performing experiments, analysis of obtained results, drawing inferences and conclude them to prepare a detailed report of positive and negative outcomes.

2. Students will be required to perform detailed study on a problem related to Experimental Chemistry or Theoretical Chemistry.

MSCH-21405 Nanochemistry

External Marks: 100 **L T P**
Internal marks: 50 **4 1 0**
Total Marks: 150

Course Objective:

1. To understand the concept of self assembly and its applications to various nano structures.
2. To understand synthesis of nano materials.
3. To learn characterization of nano materials.

1. Introduction

Introdution to nanochemistry and nanotechnology, definition & classification of nanomaterials. Properties & applications of nanomaterials. (7)

2. Self Assembly and Nanostructures

Types of self assemblies, self assembling materials. Use of self assembly in nano rod devices, nano wires, nano tubes, molecular logic gates, molecular storage devices, DNA, fullerenes, nano gas sensors. (10)

3. Nano Material Synthesis

Top down and bottom up approach, synthesis: Vapour phase synthesis by chemical routes; Nucleation & growth from solutions, stabilization against agglomeration. Processing of nano materials; Nano structured sol gel materials. Consolidation of nano crystalline materials by compaction and sintering, nanolithography. (10)

4. Characterization Techniques

Characterization of nano structured materials ï by scattering techniques, proximal microscopy (AFM & STM). (9)

5. Scope & Opportunities

Bionano composites, biometrics, nano technology enabled sensors, Microelectronics, drug delivery, bionano information. (9)

Suggested Books:

1. C.P. Poole & F.J. Owens, Introduction to Nanotechnology, Wiley, 2003.
2. M. Ratner & D. Ratner, Nanotechnology, Prentice Hall, 2003.
3. M. Wilson, K. Kannagara, G. Smith, M. Simmons & B. Raguse, Nanotechnology, CRC Press Boca Raton, 2002.

4. A. Ozin Geoffery & C. Andre, Nanochemistry, A Chemical Approach to Nanomaterials, Arsenault Royal Society of Chemists, 2005.
5. E. Foster Lynn, Nanotechnology, Science Innovation & Opportunity, Pearson Education, 2007.

MSCH-21406 Medicinal Chemistry

External Marks: 100 **L T P**
Internal marks: 50 **4 1 0**
Total Marks: 150

Course Objective:

1. To understand the concept of different types of drugs.
2. To study the synthetic route of various drugs.
3. To understand the mechanism of action of drugs.

1. Antibacterial and Antiviral Agents

History of antibacterial drugs, types, classifications, structural activity relationship, fluoroquinolones. Mechanism of action of antibacterial, ß-lactams, bacterial resistance against antibacerial drugs.

Target for anti HIV drugs, anti HIV agents, HIV-protease inhibitors, amprenavir, foseprenavir, alazanavir etc., antii-HIV nucleosides: lamivudine, retrovir, videx, hivid, zlarit, viread, carbovir, delavirdine, ziduvidine, etavirenz, calanolide, capravine, nevirapine. DNA polymerase inhibitors: acyclovir, ganciclovir, penciclovir, famicilovir, valaciclovir, valomaciclovir, codofvir (12)

2. Antimalarials

Cinchona alkaloids, 4-aminoquinolines, 8-aminoquinolines, pyramidines and sulfones, 9-aminoacridines, biguanides, mefloquine, sulfonamides.

Commercial synthetic routes to: Chloroquine, pamaquine, primaquine, proguanil, amodiaquine, mefloquine, pyremethamine, sontoquine. (8)

3. CNS Active Drugs: **CNS depressants: Hypnotics and Sedatives**

Barbiturates, non-barbiturates, amides and imides, glutethimide, benzodiazepines, aldehydes and derivatives, methaqualone and other miscellaneous agents.

Anticonvulsants: Barbiturates, hydanatoins, oxazolidinediones, succinimides, bezodiazepines, thenacemide, glutethimide.

CNS-Stimulants & Psychoactive Drugs: Analeptics, purines, psychomotor stimulants, sympathomimetics, monamine oxidase inhibitors, tricyclic antidepressants, miscellaneous psychomotor stimulants. Hallucinogens **(psychodelics, psychomimetics)**: Indolethylamines, R-phenylethylamines, butyrophenones and other miscellaneous drugs.

Commercial synthetic routes to: Thioridazine, haloperidol, chloropromazine, phenytoin, Phenobarital, Carbamazipine valproic acid, methaquolane, nitrazepam, oxazepam, diazepam, cholridazepoxide. (15)

4. Diuretics

Osmotic agents, acidfying salts .Mercurials, purines and related heterocycles, sulfonamides, benzothiadiazene and related compounds, chlorothiazides and analogs, sulfamoylebenzoic acid and analogs, endocrine antagonists, miscellaneous diuretics.

Commercial synthetic routes to: Furosemide, methalthiazide methylchlothlazide: Chlorothiazide, triameterene, hydrochlothiazide, ameloride, chlorthalidone. (10)

Suggested Books:

1. Wilson and Gisvolds Textbook of Organic Medicinal and Pharmaceuticals Chemistry, 8th edition, edited by R.F. Deorge, J.B. Lippincott Company, Philadelphia, 1982.
2. Pharmaceutical Chemicals in Perspective. B.G. Reuben and H.A. Wittcoff, John Wiley & Sons, NewYork, 1989.
3. W.O. Foye, T.L. Lamke, D.A. Williams, Principles of Medicinal Chemistry, 5th Edition, Lippencott Williams and Wilkins, 2002.

MSCH-21407 Surface Chemistry, Adsorption and Catalysis

External Marks: 100 **L T P**
Internal marks: 50 **4 1 0**
Total Marks: 150

Course Objective:

1. To understand the concept of surface chemistry.
2. To develop the understanding of aggregation processes and association of colloids.
3. To understand the phenomena of adsorption and catalysis.

1. Introduction

Basics of surface chemistry, surface tension and adsorption (4)

2. Surface & Colloid

Coagulation and kinetics of coagulation, spontaneous aging of colloids. (4)

3. Aggregation Processes

Coalescence and particle growth, Stability of colloids, Electric properties, theories of structure of electrical double layer, determination of change on colloids particle, size and shape of colloids particles. (9)

4. Association of colloids

Self - assembly system, Reversal of phase, emulsion, Macro and Micro emulsion and Aerosols, emulsifying agents, theories of emulsification, gels, sol gel transformation thixotropy. (8)

5. Electrokinetic Effect

Electrosmosis, electrophoresis, streaming potential, Dorn effect, stabilization of surfactant solutions. (8)

6. Adsorption and Catalysis

Adsorption of gases by solids, solids from solution, measurement of adsorption factors affecting adsorption, Adsorption Isotherms, Gibbs adsorption equation, surface films. Homogenous and Heterogeneous Catalysts, Acid base catalysis, Biocatalysts, Micellar catalysis, Mechanism of few catalytic reactions. (12)

Suggested Books:

1. Basic Principles of Colloids Science, D. H. Everthi, Royal Society of Chemistry, 1988.
2. Basic Physical Chemistry, W. J. Moore, Printice Hall of India, 1986.
3. Surface, G. Attard and C. Barners, Oxford Science Publications, 1998.
4. Physical Chemistry, 3rd edition , G. W Castellan, Narosa, 2002.

5. Basic and Application of Heterogeneous Catalysis, by M. Booker, Oxford Science Publication, 1998.
6. Physical Chemistry of Surfaces, A. W. Adamoson.