M.Sc. APPLIED CHEMISTRY (1ST SEMESTER)
TOTAL CONTACT HRS. = 27, TOTAL CREDITS = 23

Course		Contact Hrs.			Marks			Credits
Code	Name	L	T	P	Int.	Ext.	Total	
MCHM1-101	Electronic Spectra & Magnetic Properties of Transition Metal Complexes	3	1	0	40	60	100	4
MCHM1-102	Organic Reactions & Mechanisms-I	3	1	0	40	60	100	4
MCHM1-103	Thermodynamics	3	1	0	40	60	100	4
Departmental Elective-I		3	1	0	40	60	100	4
MCHM1-156	Computational Skills & Simulations in Chemistry							
MCHM1-157	Polymer Chemistry							
MCHM1-158	Group Theory							
Open Elective-I		3	0	0	40	60	100	3
MTEX0-F91	Textile Chemistry-I							
MMAT0-F91	Statistical Methods							
MMEE0-F91	Industrial Safety and Environment							
MCIE0-F91	Environmental Management							
MCAP0-F91	Computer Applications in Business	2	0	2				
MCHM1-104	Inorganic Chemistry Lab.-I	0	0	4	60	40	100	2
MCHM1-105	Organic Chemistry Lab.-I	0	0	4	60	40	100	2
Total 5 Theory & 2 Lab. Courses		15	4	08	320	380	700	23

M.Sc. CHEMISTRY (2nd SEMESTER)
TOTAL CONTACT HRS. = 26, TOTAL CREDITS = 23

Total Marks = 700 + 700 = 1400

Course		Contact Hrs.			Marks			Credits
Code	Name	L	T	P	Int.	Ext.	Total	
MCHM1-206	Spectroscopy-I	3	1	0	40	60	100	4
MCHM1-207	Organometallics	3	1	0	40	60	100	4
MCHM1-208	Organic Reactions & Mechanisms-II	3	1	0	40	60	100	4
MCHM1-209	Seminar-I	0	0	2	100	0	100	1
Departmental Elective-II		3	1	0	40	60	100	4
MCHM1-259	Nano Chemistry							
MCHM1-260	Bio-organic Chemistry							
MCHM1-261	Analytical Chemistry							
Departmental Elective-III		3	1	0	40	60	100	4
MCHM1-262	Bio-inorganic Chemistry							
MCHM1-263	Bio-physical Chemistry							
MCHM1-264	Asymmetric Synthesis							
MCHM1-210	Inorganic Chemistry Lab.-II	0	0	4	60	40	100	2
Total 6 Theory & 1 Lab. Courses		15	5	06	360	340	700	23

CORES OF APPLIED CHEMISTRY MRSPTU, BATHINDA		
S.No.	**Course Code**	**Course**
01	MCHM1-101	Electronic Spectra & Magnetic Properties of Transition Metal Complexes
02	MCHM1-102	Organic Reactions & Mechanisms-I
03	MCHM1-103	Thermodynamics
04	MCHM1-104	Inorganic Chemistry Lab.-I
05	MCHM1-105	Organic Chemistry Lab.-I
06	MCHM1-206	Spectroscopy-I
07	MCHM1-207	Organometallics
08	MCHM1-208	Organic Reactions & Mechanisms-II
09	MCHM1-209	Seminar-I
10	MCHM1-210	Inorganic Chemistry Lab.-II
11	MCHM1-311	Spectroscopy-II
12	MCHM1-312	Quantum Chemistry
13	MCHM1-313	Heterocyclic Chemistry
14	MCHM1-314	Seminar-II
15	MCHM1-315	Organic Chemistry Lab.-II
16	MCHM1-316	Physical Chemistry Lab.-I
17	MCHM1-417	Photochemistry
18	MCHM1-418	Natural Products
19	MCHM1-419	Physical Chemistry Lab.-I
20	MCHM1-420	Project + Seminar

DEPARTMENTAL ELECTIVES OF APPLIED CHEMISTRY MRSSTU, BATHINDA		
S.No.	**Course Code**	**Course**
DEPARTMENTAL ELECTIVE-I		
56	MCHM1-156	Computational Skills & Simulations in Chemistry
57	MCHM1-157	Polymer Chemistry
58	MCHM1-158	Group Theory
DEPARTMENTAL ELECTIVE-II		
59	MCHM1-259	Nano Chemistry
60	MCHM1-260	Bio-organic Chemistry
61	MCHM1-261	Analytical Chemistry
DEPARTMENTAL ELECTIVE-III		
62	MCHM1-262	Bio-inorganic Chemistry
63	MCHM1-263	Bio-physical Chemistry
64	MCHM1-264	Asymmetric Synthesis
DEPARTMENTAL ELECTIVE-IV		
65	MCHM1-365	Environmental Chemistry
66	MCHM1-366	Medicinal Chemistry
67	MCHM1-367	Green Chemistry

OPEN ELECTIVES OFFERED TO APPLIED CHEMISTRY MRSPTU, BATHINDA		
S.No.	**Course Code**	**Course**
OPEN ELECTIVE-I		
--	MTEX0-F91	Textile Chemistry-I
--	MMAT0-F91	Statistical Methods
--	MMEE0-F91	Industrial Safety and Environment
--	MCIE0-F91	Environmental Management
--	MCAP0-F91	Computer Applications in Business
OPEN ELECTIVE-II		
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OPEN ELECTIVES OFFERED BY APPLIED CHEMISTRY MRSPTU, BATHINDA		
S.No.	**Course Code**	**Course**
OPEN ELECTIVE-I		
91	MCHM0-F91	Oils and Fats
OPEN ELECTIVE-II		
92	MCHM0-F92	Dyes, Soaps and Detergents

F means that this Course can be opted by students of different semesters,

ELECTRONIC SPECTRA & MAGNETIC PROPERTIES OF TRANSITION METAL COMPLEXES

Subject Code: MCHM1-101 **L T P C** **Duration: 45 Hrs.**
3 1 0 4

UNIT-1

Course Objectives

1. To understand the concept of symmetry elements and symmetry operations.
2. To introduce the concept of inter electronic repulsion parameters and crystal field strength in various fields.
3. To familiarize with the Orgel and correlation diagrams.
4. To understand molecular orbital diagrams for octahedral and tetrahedral diagrams

1. Symmetry (8 Hrs.)

Symmetry elements, symmetry operations, point group determination, determination of reducible and irreducible representations, character tables, use of symmetry in obtaining symmetry of orbitals in molecules, use of character table to determine which metal orbitals are used in σ and π bond formation in octahedral, tetrahedral and square planar transition metal complexes, qualitative splitting of s, p, d, f orbitals in octahedral, tetrahedral and square planar fields using character tables and without the use of character tables.

UNIT-2

2. Inter Electronic Repulsions (7 Hrs.)

Spin-spin, orbital-orbital and spin orbital coupling, L.S. and jj coupling schemes, determination of all the spectroscopic terms of p^n , d^n ions, determination of the ground state terms for p^n , d^n , f^n ions using L.S. scheme, determination of total degeneracy of terms, order of inter electronic repulsions and crystal field strength in various fields, two type of electron repulsion parameters, term wave functions, spin orbit coupling parameters (λ) energy separation between different j states (Texts 1 and 3).

3. Free Ions in Crystal Field of various strengths (8 Hrs.)

The effect of Voct on S, P, D and F terms (with help of the character table), Strong field configurations, transition from weak to strong crystal fields, evaluation of strong crystal field terms of d^2 cases in octahedral and tetrahedral crystal fields (using group theory), construction of the correlation energy level diagrams of d^2 configuration in octahedral and tetrahedral fields, study of energy level diagrams for higher configurations, derivation of selection rules of electronic transitions in transition metal complexes, relaxation of the selection rule in centrosymmetric and non-centrosymmetric molecules, Orgel diagrams, Tanabe Sugano diagrams,

UNIT-3

4. Covalent Character into the Metal Ligand Bond (8 Hrs.)

Construction of Molecular orbital energy level diagrams for octahedral, tetrahedral and square planar complexes showing σ and π bonding. Variation of the Racah parameter, central field covalency, symmetry restricted covalency, differential radial expansion, intermediate coupling, nephlauxetic effect

UNIT-4

5. Electronic Spectra of Transition Metal Complexes (9 Hrs.)

Spectrochemical series, band intensities, factors influencing band widths (variation of 10Dq, vibrational structure, spin orbit coupling, low symmetry components, Jahn-Teller effect), discussion of electronic spectra of octahedral and tetrahedral $d^1 – d^9$ metal ions, calculation of 10Dq and B with and without the use of Tanabe Sugano diagrams, low spin complexes of

Mn^{3+}, Mn^{2+}, Fe^{3+}, Co^{3+}, Fe^{2+}, comment on the spectra of second and third transition series, Charge Transfer spectra, comparison of d – d band with f –f spectra.

6. Magnetic Properties (5 Hrs.)

General discussion about magnetism in metal complexes (magnetic susceptibility, para-, dia-, ferro-, antiferro- and ferri-magnetic behavior, Curie and Curie Weiss law, magnetic properties of *d* block transition metal ions for d^1 to d^9 configuration, quenching of orbital magnetic moment, spin only magnetic moment, first order orbital contribution to the magnetic moment, orbital contribution due to spin –orbit coupling.

Recommended Books

1. B.N. Figgis, 'Introduction to Ligand Field', Wiley Eastern, **1966**.
2. A.B.P. Lever, 'Inorganic Electronic Spectroscopy', Elsevier, **1984.**
3. R.L. Dutta and A. Syamal, 'Elements of Magnetochemistry', East-West Press Pvt. Ltd. Bangalore, **1993**.
4. J.E. Huheey & Others, 'Inorganic Chemistry: Principles of Structure and Reactivity', Harper Inter-Science, **2006.**
5. Russell S. Drago, 'Physical Method for Chemistry', W.B. Saunders Company, **1992**.
6. F.A. Cotton and G. Wilkinson, 'Advanced Inorganic Chemistry', 6th Edn., Wiley Inter-Science, **2004.**
7. F.A. Cotton, 'Chemical Application of Group Theory', 3rd Edn., Wiley Eastern, **2004**.

ORGANIC REACTION AND MECHANISM –1

Subject Code: MCHM1-102 **L T P C** **Duration: 45 Hrs.**
3 1 0 4

UNIT-1

Course Objectives

1. To familiarize with methods determining mechanism and various reaction intermediates.
2. To familiarize with diversity of aliphatic and aromatic nucleophilic and electrophilic reactions.
3. To understand the effect of substrate, leaving group, reaction medium and attacking reagent on substitution and elimination reaction.
4. To understand the concept of oxidation and auto oxidation.

1. Reaction Mechanism: Structure and Reactivity (12 Hrs.)

Type 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. Stereochemistry: Basic concepts.

UNIT-2

2. Aliphatic Nucleophilic Substitution (8 Hrs.)

The S_N2, S_N1, missed 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_Ni mechanisum, Nucleophilic substitution at an allylic,

aliphatic trigonal and a vinylic carbon. Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium, phase transferr catalysis and ultrasound, ambident nucleophile, regioselectivity. Gabriel synthesis

3. Aliphatic Electrophilic Substitution (5 Hrs.)

Bimolecular mechanisms- S_E2 and S_Ei. The S_E1 mechanism, electrophilic substitution accompanied by double bond shifts. Effect of substrates, leaving group and the solvent polarity on the reactivity, Hell-Volard-Zelinsky reaction,

UNIT-3

4. Aromatic Nucleophilic Substitution (5 Hrs.)

The S_NAr, S_N1, benzyne an $S_{RN}1$ mechanisms, Reactivity – effect of substrate structure, leaving group and attacking nucleophile. The von Richter, Sommelet-Hauser, and Smiles rearrangements.

5. Aromatic electrophilic substitution (7 Hrs.)

The arenium ion mechanism, orientation and reactivity in mono substitution and di-substituted aromatics, energy profile diagram, the ortho/para ratio, ipso attack, orientation in other ring systems, quantitative treatment of reactivity in substrates and electrophiles. Diazo coupling, Vilsmeir reaction, Gatterman-Koch reaction, Bechmann reaction, Hoben-Hoesch reaction.

UNIT-4

6. Free Radical Reactions (8 Hrs.)

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.

Recommended Books

1. Jerry March & Michael Smith, 'March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure', 6th Edn., John Wiley & Sons, **2007.**
2. Francis A. Carey & Richard J. Sundberg, 'Advanced Organic Chemistry: Structure and Mechanisms, Vol, A', 5th Edn., Springer, **2007**.
3. Francis A. Carey & Richard J. Sundberg, 'Advanced Organic Chemistry: Reaction and Synthesis', Vol. B, 4th Edn., Springer, **2006.**

THERMODYNAMICS

Subject Code: MCHM1-103 **L T P C** **Duration: 45 Hrs.**
3 1 0 4

Course Objectives

1 To recall concepts involved in laws of thermodynamics.
2 To introduce microstates, macrostates and different types statistics.
3 To recall concept of Thermodynamic equation of state.
4 To understand various thermodynamic properties and partition function.

UNIT -1

1. **Recall**: Concepts involved in first and second law of thermodynamics, Entropy, free energy and chemical equilibrium. Thermodynamic equation of state. Maxwell relations.

2. **Non-ideal Systems**: Excess functions for non-ideal systems. Activity and activity coefficients and their determination. Concept of fugacity and its experimental determination. Partial molal properties and their determination.

UNIT -2

3. **Third Law of the Thermodynamics**: Identification of statistical and thermodynamic entropy. Nernst postulate, Plank's contribution. Alternate formulation of third law. Cooling by adiabatic and demagnetisation. Evaluation of absolute entropy.
4. Thermodynamic and living systems: Simultaneous or coupled reactions. Coupled reactions and metabolism. Free energy utilisation in metabolism. Terminal oxidation chain. Overall metabolic plan. General thermodynamic consideration of living systems.

UNIT-3

5. **Statistical Thermodynamics:** General introduction, Phase space, microstates, macrostates, thermodynamic probability. Brief introduction to different types of statistics. Ensemble concept. Canonical, grand canonical and microcanocical ensembles. Stirling approximation, Maxwell Boltzmann distribution law.

UNIT-4

6. **Partition Function and Thermodynamic Properties**: Partition function and its factorization. Translational, rotational, vibrational; electronic and nuclear partition functions. Expressions for internal energy, entropy, Helmholtz function, Gibb's function, pressure, work and heat in terms of partition function. Thermodynamic properties of ideal gases. Vibrational, rotational, electronic and nuclear contributions to the thermodynamic properties.

Recommended Books

1. Aston and Fritz, 'Thermodynamic and Statistical Thermodynamics'.
2. Lee, Seers and Turcotte, 'Statistical Thermodynamics'.
3. Dickerson, 'Molecular Thermodynamics'.
4. Glasstone, 'Thermodynamics for Chemists'.
5. R.C. Srivastva, S. K. Saha, A. K. Jain, 'Thermodynamics: A Core Course', PH I, New Delhi, **2007**.
6. P. Atkins, J.D. Paula, 'Physical Chemistry', 7th Indian Edn., Oxford University Press, **2007**.
7. R.P. Rastogi & R.R. Mishra, 'An Introduction to Chemical Thermodynamics', 6th Edn., Vikas Publishing House, **2007**.

INORGANIC CHEMISTRY LAB-I

Subject Code: MCHM1-104 **L T P C**
0 0 4 2

Course Objectives

1. To develop basic understanding of various lab practices including safety measures.
2. To synthesize inorganic complexes and their characterization.

1. Preparation of coordination compounds, their purification by chromatography, elemental analyses (m, 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 $[Cr(NH_3)_6](NO_3)_3$ using magnetic susceptibility balance (MSB) and IR spectroscopy (Green Preparation).
c) Synthesis of Iron(III) dithiocarbamate and its characterization using magnetic susceptibility balance (MSB) and IR spectroscopy.

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

2. 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.

3. General Principles of Qualitative Analysis

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

4. Inorganic Analysis by using Green Methods

a) Analysis of simple acid radicals: carbonate, sulfide, sulfate, thiosulfite, chloride, bromide, iodide, nitrate.
b) Analysis of interfering acid radicals: fluoride, oxalate, borate, phosphate, arsenate, arsenite.
c) Elimination of interfering acid radicals and identifying the groups of basic radicals.
d) Analysis of basic radicals (group-wise): Lead, copper, bismuth, cadmium, tin, antimony, iron, aluminium, arsenic, zinc, manganese, nickel, cobalt, calcium, strontium, barium, magnesium, ammonium.
e) Repeating the tests in no. 04
f) Repeating the tests in no. 04
g) Analysis of a mixture-I containing three cations and three anions (of which one is interfering type).
h) Analysis of a mixture-II containing three cations and three anions (of which one is interfering type).
i) Analysis of a mixture-III containing three cations and three anions (of which one is
j) interfering type).
k) Analysis of a mixture-IV containing three cations and three anions (of which one is interfering type).

5. Complexometric Titrations

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

6. Redox Titration:

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

Recommended 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, 'Practical Inorganic Chemistry'**,** 2nd Edn., Chapman and Hall, London, **1974.**
4. J. Mendham, R.C. Denney, J.D. Barnes, M. Thomas, 'Vogel's Textbook of Quantitative Analysis', 5th Edn., Pearson Education, **2006.**
5. G. Svehla, 'Vogel's 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.

ORGANIC CHEMISTRY LAB-1

Subject Code: MCHM1-105 **L T P C**
0 0 4 2

Course Objectives

1. To impart knowledge of syntheses of organic compounds
2. To develop experimental skills of various separation and purification techniques.

1. Distillation & separation
   a) To purify common organic solvents
   b) Extract rose oil from rose petals by steam distillation.
   c) Separation of given mixtures.

2. Chromatography
   a) To separate plant pigments by column chromatography.
   b) Identification of phytoconstituents using thin layer chromatography.
   c) Identification of sugars in fruit juices through paper chromatography.

3. Organic analysis:
   Detection of common functional groups in the given organic compounds and identification of compound through derivatives.

4. Organic preparations:
   a) Benzoylation: Hippuric acid
   b) Oxidation: Adipic acid/p-Nitrobenzoic acid
   c) Aldol condensation: Dibenzalacetone/Cinnamic acid
   d) Sandmeyer's reaction: p-Chlorotoluene
   e) Benzfused Heterocycles: Benzimidazole
   f) Cannizzaro's reaction: p-Chlorobenzaldehyde as substrate
   g) Friedel Crafts reaction: S-Benzoylpropionic acid
   h) Aromatic electrophilic
   i) Substitution: p-Nitroaniline/p-Iodoaniline

Recommended Books

1. David T. Plummer, 'An introduction to Practical Biochemistry', 3rd Edn., Tata McGraw Hills, **1998**.
2. A. I. Vogel, 'Text Book of Practical Organic Chemistry', 5th Edn., Pearson Education, **2005**.
3. P.R. Singh, D.S. Gupta and K.S. Bajpai, 'Experimental Organic Chemistry', Vol 2, Tata Mc Graw Hill, **1981**.

4. G. Mann, B.C. Saunders, 'Practical Organic Chemistry', ELBS Edn,, **1989**.
5. N.K. Vishnoi, 'Advanced Practical Organic Chemistry', 2nd Edn., Vikas Publishing House Pvt. Ltd., **1994.**

COMPUTATIONAL SKILLS AND SIMULATIONS IN CHEMISTRY

Subject Code: MCHM1-156 **L T P C** **Duration: 47 Hrs.**
3 1 0 4

Course Objectives

1. To learn principles of computational chemistry and computer-based molecular design.
2. To understand the basic concepts of molecular mechanics, semi-empirical method and density-functional theory.
3. To familiarize with different software packages, including MOLDEN for general model building.
4. To understand GAMESS Gaussian for quantum chemical calculations, and BOSS for liquid simulations.

UNIT – I

1. **OVERVIEW OF THE COURSE (8 Hrs.)**
   Promises of computational chemistry, molecular mechanics of bond vibrations. Minimization methods, forces in polyatomic molecules, intermolecular forces, parameterization and testing of force fields, docking.
2. **MONTE CARLO METHOD (4 Hrs.)**
   Principles, chemical & biochemical applications.

UNIT – II

3. **MO THEORY (10 Hrs.)**
   Foundations, semi-empirical MO theory, Ab Initio MO Theory: Basis Sets; Hartree–Fock theory: Principles and applications.

UNIT – III

4. **TREATMENT OF ELECTRON CORRELATION (10 Hrs.)**
   MCSCF, CI methods, Treatment of electron correlation: MP and CC methods.

UNIT – IV

5. **SPECTROSCOPY (7 Hrs.)**
   Vibrational spectroscopy and gas phase thermodynamics, description of electronically excited states. Description of solvent effects.
6. **DENSITY FUNCTIONAL THEORY (DFT) (6 Hrs.)**
   Principles, applications in materials. Transition states in gas phase reactions.

Recommended Books

1. Peter Comba, Trevor W. Hambley, 'Molecular Modelling of Inorganic Compounds'**,** John Wiley & Sons, **2009**.
2. F. Jensen, 'Introduction to Computational Chemistry'**,** John Wiley & Sons, **1998**.
3. Warren J. Hehre, 'A Guide to Molecular Mechanics and Quantum Chemical Calculations', **2003.**
4. H.D. Holtje, W. Sippl, D. Rognan, G. Folkers, 'Molecular Modeling: Basic Principles and Applications'**,** Wiley, **2008**.
5. Christopher Cramer, 'Essentials of Computational Chemistry, Theories & Models'**,** 2nd Edn., Wiley, **2002**.

6. Note: Freely available packages like GAMESS, MOLDEN, AVOGADOOS, MOPAC may be used for computational Lab.

POLYMER CHEMISTRY

Subject Code: MCHM1-157 **L T P C** **Duration: 45 Hrs.**
3 1 0 4

Course Objectives

1. To impart knowledge about polymers and polymerization mechanism.
2. To understand the difference between crystalline and amorphous polymers.
3. To familiarize polymer characterization with various spectroscopic techniques.
4. To learn molecular weight measurement by osmometry, mass spectrometry and Viscometry.

UNIT-I

1. INTRODUCTION TO POLYMERS (6 Hrs.)
IUPAC nomenclature of vinyl, non-vinyl polymers, copolymers and end groups. Abbreviations for polymers. Introduction to industrial polymers-plastic thermoplastic- & thermosetting plastics), fibres (commonly used natural & synthetic fibre).

2. POLYMERIZATION MECHANISMS (6 Hrs.)
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.

UNIT-II

3. KINETICS OF POLYMERIZATION MECHANISMS (5 Hrs.)
Kinetics of free radical chain polymerization, ionic chain polymerization, catalyzed and non-catalyzed polycondensation polymerization including kinetic chain length, chain transfer reactions.

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

UNIT-III

5. CHEMICAL STRUCTURE & POLYMER MORPHOLOGY (5 Hrs.)
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.

6. POLYMER PROPERTIES (6 Hrs.)
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.

UNIT-IV

7. FIBRES REINFORCED POLYMER COMPOSITES (5 Hrs.)

Introduction to composites. Polymer matrix materials & fibres reinforcement. Types of fibres- glass,aramid, & silica fibres. Advantages & disadvantages of polymer composites.

8. CHARACTERIZATION TECHNIQUES OF POLYMERS (6 Hrs.)

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

Recommended 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', 3rd Edn., Oxford University Press, Indian Edn,, 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, N.V. Viswanathan, J. Sreedhar; 'Polymer Science', New Age International, **1986**.

GROUP THEORY

Subject Code: MCHM1-158 **L T P C** **Duration: 45 Hrs.**
3 1 0 4

Course Objectives

1. To educate about the importance of symmetry elements and operations.
2. To understand Great Orthogonality Theorem.
3. To develop an understanding of molecular orbital theory and ligand field theory with respect to symmetry properties.
4. To equip with the identification of IR active and Raman active vibrations and hybridization of central atom in molecule with the help of character table.

UNIT-1

1. Symmetry Elements and Operations (5 Hrs.)

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

2. Relations among Symmetry Elements (8 Hrs.)

Products of symmetry operations, equivalent symmetry elements and equivalent atoms, general relations among symmetry elements and operations, symmetry point groups, symmetry classification of elements of a Group, order of a group. Group Multiplication Table.

UNIT-2

3. Representations of Groups (8 Hrs.)

Matrix multiplication, character of matrix, Matrix notation for symmetry operations, Block factored matrices, The Great Orthogonality Theorem, Important rules about irreducible representations and their characters, relationship between reducible and irreducible representations with examples. Construction of character tables.

UNIT-3

4. Hybridization and Spectroscopy Applications (6 Hrs.)

Hybridization scheme in Sigma and Pi bonding, Identification of IR active & Raman active vibrations.

5. Molecular Orbital Theory for Inorganic Compounds (10 Hrs.)

Transformation properties of atomic orbitals, molecular orbitals for sigma bonding in tetrahedral and octahedral molecules.

UNIT-4

6. Ligand Field Theory (8 Hrs.)

Introduction, Electronic structure of free atoms and ions, splitting of levels and terms in a chemical environment, construction of energy level diagram.

Recommended Books

1. A. Salahuddin Kunju & G. Krishnan, 'Group Theory and Its Applications in Chemistry', PHI Learning Private Limited, New Delhi, **2010.**
2. F. A. Cotton, 'Chemical Applications of Group Theory', 3rd Ed., Wiley Eastern, **2004**.
3. J.N. Murell et. al, 'Valence Theory', John Wiley, **1970.**
4. R.B. Woodward and R. Hoffmann, 'Conservation of Orbital Symmetry', Academic Press, **1970.**
5. B.N. Figgis, 'Introduction to Ligand Fields', John Wiley, **1996**.

SPECTROSCOPY – I

Subject Code: MCHM1-206 **L T P C** **Duration: 45 Hrs.**
3 1 0 4

Course Objectives

1. To introduce the concept of spectroscopy, selection rules, line width and broadening.
2. To familiarize with the terms chromophores, auxochromes, red, blue, hypo and hyperchromic effect.
3. To understand vibrations of polyatomic molecules and use of group theory to determine the number of active lines.
4. To evaluate the utility of spectroscopy as a qualitative and quantitative method for structure elucidation.

UNIT-1

1. General Features of Spectroscopy (5 hrs.)

Units and conversion factors, Introduction to spectroscopy, Nature of radiation, Energies corresponding to various kinds of radiation, Intensities of spectral lines, selection rules and transition moments, Line widths, Broadening (Book 1)

UNIT-2

2. Pure Rotational Spectra (10 Hrs.)

Classification of molecules according to their moment of inertia. Rotational energy levels of hydrogen chloride. Determination of molecular geometry by rotational spectrum, isotopic substitution effects. Stark effect, Estimation of molecular dipole moments, Selection rules,

Rotational Raman Spectra, anisotropic polarizability, specific selection rule in Raman Spectra, Stokes and anti – Stokes lines.

3. Vibrational Spectra (5 Hrs.)

Diatomic molecules, Force constants, Fundamental vibration frequencies, Anharmonicity of molecular vibrations and its effect on vibrational frequencies, Frequencies of the vibrational transitions of HCl. Vibrational rotation spectra of CO, P, Q and R branches.

UNIT-3

4. Infrared and Raman Spectra (15 Hrs.)

Vibrations of polyatomic molecules. Examples of CO_2, H_2O. Mechanics of measurement of infrared and Raman spectra, absorption of common functional groups, their dependence on chemical environment (bond order, conjugation, H – bonding), Use of group theory to determine the number of active infrared and Raman active lines. Fermi resonance, combination bands and overtones, Application of IR in structure elucidation of organic compounds – Various Carbonyl compounds, alkane, alkenes, alkynes, unsubstituted, mono and di-substituted aromatic compounds, alcohols, phenols, ethers, Far IR region, Metal ligand vibrations, – CN, Nitro-nitrito- and CO ligands and the effect of their co-ordination with metal ions and IR spectra.

UNIT-4

5. UV and Visible Spectroscopy of Organic Molecules (10 Hrs.)

Measurement technique, Beer – Lambert's Law, molar extinction coefficient, oscillator strength and intensity of the electronic transition, Frank Condon Principle, Ground and first excited electronic states of diatomic molecules, relationship of potential energy curves to electronic spectra. Chromophores, auxochromes, electronic spectra of polyatomic molecules, Woodward rules for conjugated dienes and α, β- unsaturated carbonyl groups, extended conjugated and aromatic sterically hindered systems, red shift, blue shift, hypo- and hyperchromic effect.

Recommended Books

1. Russell S. Drago, 'Physical Method for Chemistry', 2nd Edn., Surfside Scientific Publishers, **1992.**
2. R.M. Silverstein, G.C. Bassler, T.C. Morrill, 'Spectrometric Identification of Organic Compounds', 3rd Edn.,, Wiley, **1974**.
3. William Kemp, 'Organic Spectroscopy', 3rd Edn., W.H. Freeman, **1991**.
4. Dudley H. Williams & Ian Fleming, 'Spectroscopic Methods in Organic Chemistry', 6th Edn., McGraw-Hill, Science, **2008.**
5. J.R. Dyer, 'Application of Absorption Spectroscopy of Organic Compounds' Prentice-Hall, Englewood Cliffs, N.J., **1965**.
6. Dudley H. Williams & Ian Fleming, 'Spectroscopic Problems in Organic Chemistry' 5th Edn., McGraw-Hill, London, **1985**.
7. R.C. Banks, E.R. Matjeka, G. Mercer, 'Introductory Problems in Spectroscopy' Manlo Park, CA, **1980**.
8. G.M. Barrow 'Introduction to Molecular Spectroscopy' McGraw-Hill, New York, **1962**.
9. C.N. Banwell 'Fundamentals of Molecular Spectroscopy' 4th Edn., Tata McGraw-Hill Education, **1994**.
10. D.L. Pavia, G.M. Lampan and G. S. Kriz, 'Introduction to Spectroscopy', 4th Edn., Cengage Learning, **2008**.

ORGANOMETALLICS

Subject Code: MCHM1-207 **L T P C** **Duration: 45 Hrs.**
3 1 0 4

Course Objectives

1. To recall classification of ligands and nomenclature of organometallic compounds.
2. To understand structure, bonding and reactivity of organometallic compounds.
3. To familiarize with the role of organometallic compounds in organic syntheses.
4. To understand the applications of organometallic compounds as catalysts.

UNIT-1 (11 Hrs.)

1. Introduction- Stability & decomposition pathways, classification of ligands, nomenclature of Organometallic compounds.
2. 18 valence electron rule- Introduction to the 18 valence electron rule, total electron counts and finding metal-metal bonds & related problems.

UNIT-2 (11 Hrs.)

3. Synthesis, structure, bonding & reactivity of organotransition metal complexes.
   (i) Carbenes, Carbynes, Alkenes, Alkynes, Allyl moieties, Butadiene, Cyclobutadiene, Cyclopentadiene, Arenes, Cycloheptadienyl moieties & Cyclo octatetraene moieties, Ring slippage reactions.
   (ii) Ferrocenes- Structure & bonding of ferrocenes, basic chemical reactions of ferrocenes, chirality in ferrocene derivatives, ferrocene based condensation polymers.

UNIT-3 (10 Hrs.)

4. Organometallic compounds in organic Synthesis-Green rules, synthesis & use of Zinc dialkyls, Collaman's reagent, organ mercuric & chromium carbonyls in organic synthesis, Heck reaction, Hydrozirconation.

UNIT-4 (13 Hrs.)

5. Applications of organometallic complexes to Catalysis-Basic principles, Industrial requirements of catalysts, sequences involved in catalytic reaction, asymmetric synthesis using catalyst, Hydrogenation catalysts & their classification, hydrogenation by lanthanide organometallic compounds. Hydro formylation: Cobalt catalyst & phosphine modified cobalt catalysts, Rhodium-phosphine catalysts, factors affecting n/iso ratio of hydro formylation products. Monsato, Cativa & Wacker processes, polymerization & oligomerisation of olefins & dienes, catalytic converters.

Recommended Books

1. 'Basic Organometallic Chemistry: Concepts, Synthesis & Application of Transition Metals', CRC Press & Univ. Press, **2010**.
2. R.C. Mehrotra & A, Singh, 'Organometallic Chemistry, A Unified Approach', New age International.
3. B.D. Gupta & A.J. Elias, 'Basic Organometallic Chemistry', Universities Press.
4. F.A. Cotton & G. Wilkinson, 'Advanced Inorg, Chemistry', Wiley Intersciences.

ORGANIC REACTION AND MECHANISMS –1I

Subject Code: MCHM1-208 **L T P C** **Duration: 45 Hrs.**
3 1 0 4

Course Objectives

1. To extend knowledge of mechanistical and stereochemical aspects of organic reactions.
2. To impart knowledge of various oxidative and reductive processes in organic syntheses.

3. To understand the mechanism of various organic reactions including Beckmann, Neber, Hofmann, Schmidt and Fries rearrangement.
4. To familiarize with syntheses of prostaglandins, strychnine, reserpine and biotin etc.

UNIT-1

1. Addition to Carbon-Carbon and Carbon-Hetero Multiple Bonds (10 Hrs.):

Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, regio- and chemoselectivity, orientation and reactivity. Addition to cyclopropane ring. Hydrogenation of double and triple bonds, hydrogenation of aromatic rings. Hydroboration. Michael reaction. Sharpless asymmetric epoxidation. Addition of Grignard reagents, organozinc, organolithium and Gillman reagents to carbonyl and unsaturated carbonyl compounds. Use of other organometallic reagents in addition reactions. Wittig reaction, Mechanism of condensation reactions involving enolates – Aldol,.Knoevenagel, Claisen, Mannich, Benzoin, Perkin and Stobbe reactions. Hydrolysis of esters and amides, ammonolysis of esters.

UNIT-2

2. Elimination Reactions (5 Hrs.):

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

3. Oxidation (7 Hrs.):

Introduction. Different oxidative processes. Hydrocarbons- alkenes, aromatic rings, saturated C-H groups) activated and inactivated). Alcohols, diols, aldehydes, ketones, ketals and carboxylic acids. Amines, hydrazines, and sulphides.

Oxidations with ruthenium tetraoxide, iodobenzene diacetate and thallium (III) nitrate, DDQ, PCC, CAN, selenium dioxide, peroxyacids, DCC. Oxidation reactions with special emphasis on Baeyer-villeger reaction, Cannizarro oxidation-reduction reaction,

UNIT-3

4. Reduction (10 Hrs.):

Introduction. Different reductive processes, Hydrocarbons- alkanes, alkenes, alkynes and aromatic rings, Carbonyl compounds – aldehydes, ketones, acids, ester and nitriles. Epoxides, Nitro, nitroso, azo and oxime groups, Hydrogenolysis. Sodium borohydride, sodium cyano borohydride, LAH, disobutyl aluminium hydride, tin hydride, trialkyl tin hydride, trialkyl silanes, alkoxy substituted LAH, DIBAL, diborane, diisoamyl borane, hexyl borane, 9-BBN, isopinocamphenyl and disiopinocamphenyl borane. Reduction reactions with particular emphasis on Wolf-Kishner reduction, Clemmensen reduction,

UNIT-4

5. Rearrangements (8 Hrs.):

General mechanistic consideration – 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, Shapiro reaction, Fries rearrangement

6. Selected Natural Product Synthesis (5 Hrs.)

Corey's synthesis of prostaglandins (PGF2 and PGE2), Woodward synthesis of Strychnine and Reserpine, Synthesis of Biotin by Hoffman-LaRoch, synthesis of Indolizomycin by Danishefsky, Synthesis of Taxol by K.C. Nicolau.

Recommended Books:

1. Jerry March & Michael Smith, 'March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure', 6th Edn., John Wiley & Sons, **2007**.

2. Francis A. Carey & Richard J. Sundberg, 'Advanced Organic Chemistry: Structure and Mechanisms, Vol, A', 5th Edn., Springer, **2007**.
3. Francis A. Carey & Richard J. Sundberg, 'Advanced Organic Chemistry: Reaction and Synthesis, Vol. B', 4th Edn., Springer, **2006.**
4. K.C. Nicolaou and E.J. Sorensen, 'Classics in Total Synthesis: Targets, Strategies, Methods', Wiley, **1996**.

SEMINAR-I

Subject Code: MCHM1-208 **L T P C** **Duration: 22 Hrs.**
0 0 2 1

1. Each of these Courses of Seminar will consist of 100 marks (internal only) having L T P C as 0 0 2 1.
2. In the beginning of the semester, a teacher will be allocated maximum 30 students. The latter will guide/teach them how to prepare/present 15 minutes Power Point Presentation for the Seminar.
3. If there are more than 30 students in the class, then class will be divided into two groups having equal students. Each group may be allocated to a different teacher.
4. Each student will be allotted a topic by the teacher at least one week in advance for the presentation. The topic for presentation may be from the syllabus or relevant to the syllabus of the programme.
5. During the presentation being given by a student, all the other students of his/her group will attend the Seminar. The assessment/evaluation will be done by the teacher. However, Head of Department and other faculty members may also attend the Seminar, ask questions and give their suggestions.
6. This is a turn wise continuous process during the semester and a student will give minimum two presentations in a Semester.
7. For the evaluation, the following criteria will be adopted,
   (a) Attendance in Seminar: 25 Marks
   (b) Knowledge of Subject along with Q/A handling during the Seminar: 25 Marks
   (c) Presentation and Communication Skills: 25 Marks
   (d) Contents of the Presentation: 25 Marks.

INORGANIC CHEMISTRY LAB-II

Subject Code: MCHM1-210 **L T P C**
0 0 4 2

Course Objectives

1. To extend knowledge of use of standard laboratory equipment, modern instrumentation and classical techniques to carry out experiments.
2. To synthesize various inorganic complexes and their qualitative determination by UV, IR, NMR and ESR techniques.

1. **Reaction of Cations and Anions**: Analysis of mixture of cations and anions.
2. **Gravimetric Analysis of Cations and Anions:** Iodide, thiocyanate, Sulphate, oxalate chloride, nickel, copper cobalt, zinc and their mixture.
3. **Preparation of Inorganic and Coordination compounds**, their purification, elemental analyses, M.W determination and elucidation of structures by physical methods:
   a) Synthesis of nitro- and nitritopentamminecobalt(III) chlorides.

b) Synthesis of hexamminecobalt(III) chloride and pentammineaquocobalt(III) chloride.
c) Synthesis of cis and trans potassiumdioxalatodiaquochromate(III).
d) Aquation of trans-dichlorobis(1,2-diaminoethane)cobalt(III) chloride.
e) Synthesis and resolution of tris(ethylenediamine)cobalt(II) ion.
f) Synthesis of hexaamminenickle(II) chloride and estimation of Ni (II) in the complex by gravimetry and volumetry.
g) Synthesis of tris(acetylacetanonato)iron(III).
h) Synthesis and reactivity of organocobaloximes.
i) Synthesis of acetylferrocene and its purification by column chromatography.
j) Synthesis of ferrocene carboxylic acid.

4. Determination of Metal Ions Using Solvent Extraction:
a) Determination of copper as the diethydithiocarbamate complex
b) Determination of copper as the neocuproin complex
c) Determination of iron as the 8hydroxyquinolate
d) Determination of nickel as the dimethylglyoxime complex,
e) Extraction and determination of lead, cadmium, and copper using ammonium pyrollidine dithiocarbamate.

5. Electro Analytical Techniques
pHmetric, Conductometric and Amperometric Titration: Representative acid/base and redox titrations.

6. Colorimetry and Spectrophotometry
a) Determination of λ_{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.

7. 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.

8. Qualitative determination by UV, IR, NMR, ESR.

Recommended 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, 'Practical Inorganic Chemistry', Chapman and Hall, London, **1968**.
4. J. Mendham, R.C. Denney, J.D. Barnes, M. Thomas, 'Vogel's Textbook of Quantitative Analysis', Pearson Education, **2006.**
5. G. Svehla, 'Vogel's Textbook of Quantitative Analysis', Pearson Education, **2006**.
6. Anil J. Elias, 'A Collection of Interesting General Chemistry Experiments', University Press, **2002.**

Note: The students are required to perform atleast 2 experiments from each section.

NANOCHEMISTRY

Subject Code: MCHM1-259 **L T P C** **Duration: 45 Hrs.**

3 1 0 4

Course Objectives

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.
4. To understand the applications of nano materials in biological system.

UNIT-1

1. Introduction (5 Hrs.):

Introduction to nanochemistry and nanotechnology, definition & classification of nanomaterials. Properties & applications of nanomaterials.

2. Self-Assembly and Nanostructures (10 Hrs.):

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.

UNIT-1I

3. Nano Material Synthesis (10 Hrs.):

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.

UNIT-1II

4. Characterization Techniques (15 Hrs.):

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

UNIT-1V

5. Applications (5 Hrs.):

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

Learning Outcomes:

1. Introduction to the concept of nanochemistry and its classification and terminology.
2. Synthesis of nanomaterials by different routes and their characterization.
3. Applications in biological and electronic systems.

Recommended 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**.

BIO-ORGANIC CHEMISTRY

Subject Code: MCHM1-260 **L T P C** **Duration: 45 Hrs.**

3 1 0 4

Course Objectives

1. To illustrate the link between organic chemistry and biochemistry by discussing the organic chemistry of selected processes of living systems.
2. To integrate the chemical principles with biological applications with examples drawn from biochemistry, molecular and cell biology.
3. To understand the mechanism of enzyme catalysis.
4. T understand the mechanism of combinatorial synthesis in medicinal chemistry.

UNIT-1 (11 Hrs.)

Amino Acids and Proteins: Structure, classification, synthesis and properties of amino acids, isoelectric point, biosynthesis of amino acids. Peptides: oligo- and polypeptides, geometry of peptide linkage, N-terminal and C-terminal residue analysis, synthesis of peptides-amino and carboxyl protecting groups-solid phase peptide synthesis. Proteins: classification and properties (denaturation, isoelectric point and electrophoresis), primary, secondary, tertiary and quaternary structures of proteins, collagen and triple helix.

UNIT-II (11 Hrs.)

Enzymes and Cofactors: Mechanism of enzyme catalysis, Factors influencing enzyme action, Examples of typical enzyme mechanisms: chymotrypsin, ribonuclease and lysozyme, Enzyme-catalyzed addition, elimination, condensation, carboxylation and decarboxylation, isomerization, group transfer and rearrangement reactions-structure and biological functions of coenzyme A, thiamine pyrophosphate, pyridoxal phosphate, NAD+, NADP+, FMN, FAD, lipoic acid and Vitamin B12. Mechanisms of reactions catalyzed by the above cofactors.

UNIT-III (12 Hrs.)

Nucleic Acids and Protein Synthesis: Nucleotides and nucleosides, DNA: primary and secondary structure-replication of DNA. RNA and protein synthesis: Messenger RNA synthesis-transcription, Ribosomes-rRNA, Transfer RNA, genetic code translation. Determination of base sequence of DNA. Polymerase Chain Reaction (PCR). Antisense technology in chemotherapy and other nucleic acid-targeted drugs-intercalates, sequence specific drugs. A brief account of ribozyme and iRNA.

UNIT-IV (11 Hrs.)

Lead and Analogue Synthesis-1: Designing organic synthesis-disconnection approach-synthons and synthetic equivalents-one group disconnections: alcohol, olefin, ketone, acids-two group disconnections:1,2-, 1,3-, 1,4- and 1,5-difunctional compounds-convergent synthesis-functional group interconversions- functional group additions-carbon heteroatom bonds-methods for 3- to 6-membered rings.

Lead and Analogue Synthesis-2: Combinatorial synthesis in medicinal chemistry: Solid phase techniques-methods of parallel synthesis-mix and split techniques-dynamic combinatorial chemistry-screening and deconvolution-limitations of combinatorial synthesis Asymmetric synthesis: basic principles-stereo selective and stereospecific reactions- methods for determining enantiomeric excess-chiral auxiliary, reagents and catalysts and their applications (wherever applicable) in alkylation, hydrogenation, hydroxylation, epoxidation and hydroboration of alkenes, reduction of ketones-Cram and Felkin-ahn models. Noyori's BINAP – Jacobson catalyst – Evans catalyst.

Recommended Books:

1. Hermann Dugas and C. Penny, 'Bioorganic Chemistry: A Chemical Approach to Enzyme action', Springer-Verlag.
2. N.C. Price and L. Stevens, 'Fundamentals of Enzymology', Oxford University Press.
3. C. Walsh, W.H. Freeman, 'Enzymatic Reaction Mechanisms'.

4. Stuart Warren, 'Designing Organic Synthesis: The Disconnection Approach', 2nd Edn., Wiley, **1984**.
5. H.B. Kagan, 'Asymmetric Synthesi', Thieme Medical Publishers, **2003**.
6. Francis A. Carey and Richard B. Sundberg, 'Advanced Organic Chemistry: Part-A and Part-B', 5th Edn., Springer, **2007**.

ANALYTICAL CHEMISTRY

Subject Code: MCHM1-261 **L T P C** **Duration: 45 Hrs.**
3 1 0 4

Course Objectives

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 analysing the chemicals applying the electroanalytical and thermogravimetric instruments.
4. To know the methods of separating the mixture of compounds by chromatographic Techniques.

UNIT-1

1. Introduction to Analytical Chemistry

Types of analytical methods: Importance of analytical methods in qualitative and quantitative analysis: chemical and instrumental 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.

2. Thermoanalytical Techniques

Principle of thermogravimetry, differential thermal analysis, differential scanning calorimetry - instrumentation for TGA, DTA and DSC-characteristics of TGA and DTA curves - factors affecting TGA and DTA curves. Applications of thermal analysis.

UNIT-2

3. Electrochemical Techniques

Basic principle, instrumentation and applications of cyclic voltametry and coulometry, potentiometery, voltametry**,** polarography.

4. High Performance Liquid Chromatography

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

UNIT-3

5. Microscopy Techniques

Basic principle, instrumentation and applications of electron microscopy - SEM, TEM, scanning probe microscopy – AFM.

6. X- Ray Diffraction

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

UNIT-4

7. Neutron Diffraction

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

8. Electron Diffraction

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

Recommended Books:

1. A Douglas, Skoog and Donald M. West, F.J. Holler, 'Fundamentals of Analytical Chemistry', 8th Edn., Harcourt College Publishers, **2004**.
2. Skoog, Holder, Nieman, 'Principles of Instrumental Analysis', 5th Edn., Thomson Books, **1998**.
3. J. Mendham, R.C. Denney, J.D. Barnes, M. Thomas, 'Vogel's Text Book of Quantitative Chemical Analysis', 6th Edn., Pearson Education, **2006**.
4. R. Gopalan, P.S. Subramaniam and K. Rengarajan, 'Elements of Analytical Chemistry', 3rd Edn., 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 Edn., 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 Edn., Oxford, **2006**.
9. A. Braithwaite and F.J. Smith, 'Chromatographic Methods', 5th Edn., Blackie Academic and Professional, London, **1996**.

BIO-INORGANIC CHEMISTRY

Subject Code: MCHM1-262 **L T P C** **Duration: 48 Hrs.**
3 1 0 4

Course Objectives

1. To understand structures, processes and chemical interactions of enzymes with metal ions in biological systems.
2. To understand the transport mechanisms of enzymes in physiological systems.
3. To acquire knowledge of metal complexes with various nucleic acids.
4. To study the role of metal complexes in transcription of nucleic acid.

UNIT-I & UNIT-II

1. Inorganic Chemistry of Enzymes (30 Hrs.)

Introduction, non-photosynthetic processes, metallo-porphyrines, cytochromes, biochemistry of iron, iron storage and transport, ferritin transferring, bacterial iron transport, haemoglobin and myoglobin, nature of heme-dioxygen binding, model systems, cooperativity in haemoglobin, physiology of myoglobin and haemoglobin, structure and function of haemoglobin.

Structure and function, inhibition and poisoning Vitamin B_{12} and B_{12} coenzymes metallothioneins, nitrogen fixation, in-vitro and in-vivo nitrogen fixation, bio-inorganic chemistry of Mo and W, nitrogenases: other elements V, Cr, Ni (essential and trace elements in biological systems).

Other iron-prophyrin biomolecules, structure and function of hemoglobin. Other iron-porphyrin biomolecules, peroxidases and catalases, cytochrome P450 enzymes, other natural oxygen carriers, hemerythrins, electron transfer, respiration and photosynthesis; ferridoxins, and subredonim carboxypeptidase, carbonic anhydrase, metallothioneins.

UNIT-III & UNIT-IV

2. Metal Ions in Biological Systems (18 Hrs.)

Metal complexes of polynucleotides, nucleosides and nucleic acids (DNA & RNA). Template temperature, stability of DNA.

Role of metal ions in replication and transcription process of nucleic acids. Biochemistry of calcium as hormonal messenger, muscle contraction blood clotting, neurotransmitter, calcification reclaiming of barren land. Metals in the regulation of biochemical events. Transport and storage of metal ions *in vivo*.

Course Learning Outcomes

1. Structures, properties and transport mechanisms of enzymes in physiological systems
2. Metal complexation with various nucleic acids and their role in transcription of nucleic acids

Recommended Books

1. J.E. Huheey, E.A. Keiter and R.L. Keiter, 'Inorganic Chemistry: Principles of Structure and Reactivity', 4th Edn., Haper Collins.
2. B. Douglas, D. McDaniel and J. Alexander, 'Concepts and Models of Inorganic Chemistry', 3rd Edn., John Wiley and Sons.
3. F.A. Cotton and G. Wilkinson, 'Advanced Inorganic Chemistry: A Comprehensive Text', 5th Edn., John Wiley.
4. Ch. Elschenbroich and A. Salzer, 'Organometallics. A Concise Introduction', 2nd Edn., VCH.
5. D.F. Shriver and P.W. Atkins, 'Inorganic Chemistry', 3rd Edn., Oxford University Press.
6. J.A. Cowan, 'Inorganic Biochemistry', 2nd Edn., Wiley-VCH.
7. G. Wulfsberg, 'Inorganic Chemistry', University Science Books.
8. S.J. Lippard & J.M. Berg, 'Principles of Bioinorganic Chemistry', Univ. Science Books, **1994**.
9. S.J. Lippard, 'Progress in Inorganic Chemistry', Vols. 18, 38, Wiley-Interscience, **1991**.

BIO-PHYSICAL CHEMISTRY

Subject Code: MCHM1-263 **L T P C** **Duration: 43 Hrs.**
3 1 0 4

Course Objectives

1. To equip with basic knowledge of the physical principles that governs chemical systems.
2. To provide knowledge of various biological systems with emphasis on biochemical reactions.
3. To recall enzymes, their role in chemical and biological catalysis.
4. To understand various principles that govern cellular processes.

UNIT-1

Biological Cell and its Constituents (4 Hrs.):

Biological cell, DNA and RNA in living systems. Basic consideration. Proximity effects and molecular adaptation.

Enzymes (6 Hrs.):

Introduction and historical perspective, chemical and biological catalysis, Remarkable properties of enzymes like catalytic power, specificity and regulation. Nomenclature and classification, extraction and purification. Fischer'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 Line Weaver-Burk plots, reversible and irreversible inhibition.

UNIT-2

Kinds of Reactions Catalyzed by Enzymes (5 Hrs.):
Nucleophilic displacement on a phosphorus atom, multiple displacement reactions and the coupling of ATP cleavage to endergonic processes. Transfer of sulphate, addition and elimination reaction, enolic intermediates in isomerization reactions, b-cleavage and condensation, some isomerization and rearrangement reactions. Enzyme catalyzed carboxylation and decarboxylation.

Co-Enzyme Chemistry (5 Hrs.):
Cofactors as derived from vitamins, coenzymes, prosthetic groups, apoenzymes. Structure and biological function of coenzyme A, thiamine pyrophosphate, Pyridoxal phosphate, NAD+, NADP+, FMN, FAD, lipoic acid, vitamin B12. Mechanism of reaction catalyzed by the above cofactors.

UNIT 3

Biological Macromolecules (4 Hrs.)
The Nucleic Acids: Nucleotide, torsion angles in poly nucleotide chains, the helical structure of polynucleic acids, high order structure in polynucleotides.

Interactions in Macromolecules: (4 Hrs.)
Basic principles of interaction between molecules, water structure and its interaction with biomolecules, dipole interactions, side chain interactions, electrostatic interactions, base pairing in nucleic acids, base stacking, hydration and the hydrophobic effect.

Structural Transition in Bio-macromolecules (3 Hrs.):
Coil – helix transitions in proteins, statistical methods for predicting protein secondary structures; melting and annealing of polynucleotide duplexes, helical transitions in double stranded DNA, super coil dependent DNA transitions predicting helical structures in genomic DNA.

UNIT-4

Bioenergetics and ATP cycle (8 Hrs.)
Standard free energy change in biochemical reaction, exergonic, endergonic reactions. Hydrolysis of ATP, synthesis of ATP from ADP, metal complexes and transition of energy, chlorophylls, photo system I and photo system II in cleavage of water.

Thermodynamics of Biopolymer Solutions (4 Hrs.)
Thermodynamics of biopolymers solutions, osmotic pressure, membrane equilibrium, muscular contraction and Energy generations in mechano-chemical system.

Recommended Books:

1. A.L. Lehninger, 'Principles of Biochemistry', Worth Publishers.
2. Voet; 'Voet Biochemistry', John Wiley, **1995**.
3. E.E. Conn, P.K. Stumpt, 'Outlines of Biochemistry', John Wiley.
4. Hermann Dugas, C. Penny, 'Bio-organic Chemistry: Chemical Approach to Enzyme Action', Springer Verlag, **1982**.
5. M.I. Page, A. Williams, 'Enzyme Mechanisms,' Royal Society of Chemistry.
6. Richard B. Silverman, 'Organic Chemistry of Enzyme Catalysed Reaction'.
7. I. Bertini, H.B. Gray, S.J. Lippard, J.S. Valentine, 'Bioinorganic Chemistry', University Science Books.
8. William Jolley, 'Bioinorganic Chemistry'.

9. K.E. Van Holde, W.C. Johnson, P.S. Ho, 'Principles of Physical Biochemistry', Prentice Hall,**1998**.
10. L. Stryer, 'Biochemistry', W.H. Freeman.
11. J. David Rawn, 'Biochemistry', Neil Patterson.
12. F. Wold, 'Macromolecules: Structure and Function', Prentice Hall.
13. C.R. Cantor, P.R. Schimmel, 'Biophysical Chemistry', Vol. 1-3, Freeman, **1980**.

ASYMMETRIC SYNTHESIS

Subject Code: MCHM1-264 **L T P C** **Duration: 45 Hrs.**
3 1 0 4

Course Objectives

1. To learn the theory and importance of asymmetric Synthesis.
2. To acquire knowledge about various Principles of asymmetric Synthesis.
3. To give an understanding of various methods of asymmetric Synthesis.
4. To know the methods of separating the mixture of meso-compounds by various techniques.

UNIT – I

1. Basic Principles of Asymmetric Synthesis (10 Hrs.)

Definition: (enantiotropic and diast- ereotropic) groups and faces – Symmetry, substitution and addition criteria. Prochirality nomenclature: Pro – R, Pro – S, Re and Si.
Selectivity in synthesis: Stereospecific reactions (substrate stereoselectivity), Srereo selective reaction (Product stereoselectivity), Enantioselectivity and diastereoselectivity.
Conditions of Stereoselectivity: Symmetry and transition state criteria, kinetic and thermodynamic control. Methods for inducing enantio- and diastereoselectivity.

UNIT – II

2. Analytical Methods (10 Hrs.)

Determining % Enantiomer excess, % Enantioselctivity, Optical Purity, % Diastereomeric excess and % diatereoselectivity. Resolving agents and resolution of racemic compounds having common functional groups e.g. alcohol, amine, acid. Techniques for determination of Enantioselectivity. Specific rotation; Chiral ^{1}NMR, Chiral lanthanide shift reagents and chiral HPLC.

UNITS – III & IV

3. Classification of Asymmetric Reactions (25 Hrs.)

i) Substrate controlled asymmetric synthesis: Nucleophilic addition to chiral carbonyl compounds, 1,2 –Asymmetric induction, Cram's rule and Felkin-Anh model, Double stereo differentiation; matched pair and mismatched pair, Examples from aldol condensation and hydroboration reactions
ii) Chiral auxiliary controlled asymmetric synthesis: α-alkylation of chiral enolates, azaenolates, imines and hydrazones, chiral sulphoxides.
1,4-asymmetric induction and Prelog's rule, use of chiral auxiliary in Diels-Alder and Cope reactions.
iii) Chiral reagent controlled asymmetric synthesis: Asymmetric reduction using BINAL-H. Asymmetric Michael addition to α, β-unsaturated carbonyl compounds, Chiral lithium amides- enantioselective deprotonation, applications of chiral organoboranes.
iv) Chiral catalyst controlled asymmetric synthesis: Sharpless, Jacobson and Shi asymmetric epoxidation, Sharpless asymmetric dihydroxylation and amino hydroxylation. Asymmetric hydrogenations using chiral Wilkinson biphosphine and Noyori catalyst. Chiral catalyst

controlled Diels-Alder and Michael reactions, Utility metal-semicorrinato complexes and Jacobson Catalysts-Evans Catalyst- Aziridination, Enzyme mediated enantioselective synthesis.

Recommended Books

1. J.D. Morrison and H.S. Moscher, 'Asymmetric Organic Reactions', Vol 1-5, Academic Press, **1983.**
2. E.N. Jacobsen, A. Pfaltz, H. Yamamoto, 'Comprehensive Asymmetric Catalysis' Eds. Springer, **2000.**
3. Nogardi, 'Asymmetric Synthesis'.
4. R.S. Ward, 'Stereoselectivity in Organic Molecules', Wiley, New York, **1999**.
5. Y. Izumi, 'Stereo Differentiating Reactions', Academic Press, **1977.**
6. E.L. Eliel, 'Stereochemistry of Carbon Compounds' Wiley, **1992**.
7. W. Carruthers, 'Some Modern Methods of Organic Synthesis', 4th Edn., Cambridge University Press, **2012.**
8. I. Ojima, 'Catalytic Asymmetric Synthesis', VCH-NY, Pergamon, **1998.**
9. R.E. Gawley, J. Aube, 'Principles of Asymmetric Synthesis', (Tetrahedron Series in Organic Chemistry), Pergamon, **1996.**
10. H.B. Kagan, 'Asymmetric Synthesis', Edn., I, Thieme Medical Publishers, **2003**.
11. G. Proctor, 'Asymmetric Synthesis', Oxford University Press, USA, **1997**.