

**MADRAS CHRISTIAN COLLEGE (Autonomous)**

**Department of Chemistry**

**Master of Science in Chemistry**

Regulations and Syllabi

(Effective from July 2002)

**1. Eligibility for admission:**

- A candidate who has passed the B.Sc. degree examination in chemistry main with ancillary mathematics of Madras University or an autonomous college or an examination of some other University accepted by the Senates of Madras Christian College as equivalent thereto shall be permitted to appear and qualify for M.Sc. in Chemistry examination of this college after a course of study of two academic years comprising two semesters a year.

**2. Duration of the course:**

- The course for the degree of M.Sc. shall consist of four semesters, two in the first and two in the second year.

**3. End of semester examinations:**

- For purposes of these regulations, the academic year shall be divided into two semesters, the first is from June to November and the second from December to May. The end of semester examination in the first semester will be conducted in November/December and the examinations in the second semester in April/May. Likewise, the examinations in third and fourth semesters will be conducted in November/December and April/May.
- A candidate who does not pass the examination in any subject or subjects of the first, second and the third semesters will be permitted to appear in such failed subjects alone with other subsequent semester examinations. For the failed candidates in each semester the examination will be held in both May/June and November/December.

**4. Continuous assessment (CBCS pattern) :**

- There will be two tests for each subject during each semester. Each test will be for a maximum of 50 marks. Marks of both performances will be considered for awarding the 50 marks in each subject towards the continuous assessment.
- However if the student so desires, he/she may write a third continuous assessment test for the entire syllabus, which will also be for a maximum of 50 marks. For computing the continuous assessment marks the two best performance will be considered.

**5. Practicals:**

- The syllabus for each subject for each semester is an independent unit which must be completed during that semester. The continuous assessment for each semester in each subject will be for a total of 50 marks, according to the following scheme:

Quantum of work .. .. .	20
Accuracy in selected experiments ..	25
Record .. .. .	5

- Six experiments in each semester in each subject for testing the students' skill in obtaining accurate results. Out of these, four best performances will be considered for awarding the 25 marks for accuracy. A student should be considered for the award of the full 20 marks for quantum of work only if he completes all the experiments prescribed in the syllabus. The marks for the records will be awarded based on regularity of submission and neatness.
- NO END OF SEMESTER PRACTICAL EXAMINATIONS WILL BE HELD.

## 6. Details of Courses and Examinations:

Sem.	Paper	Title	Weekly hours	Exam hours	Marks		Credits
					CA	ESE	
I	MC01	Basic Concepts in Organic Chemistry(C)	5	3	50	50	4
	MC02	Materials Science(C)	5	3	50	50	4
	MC03	Thermodynamics and Chemical Kinetics(C)	5	3	50	50	4
	MC04	Environmental Chemistry (E)	5	3	50	50	5
	MC05	Practicals I (Organic Chemistry Practicals – I + Inorganic Chemistry Practicals – I + Physical Chemistry Practicals – I)	10	-	50	-	4
	MC06	Seminar I	-	-	25	-	1
II	MC07	Organic Reaction Mechanism(C)	5	3	50	50	4
	MC08	Analytical Techniques in Chemistry(C)	5	3	50	50	4
	MC09	Group theory and Quantum Mechanics(C)	5	3	50	50	4
	MC10	Polymer Chemistry (E)	5	3	50	50	5
	MC11	Practicals II(Organic Chemistry Practicals – II + Inorganic Chemistry Practicals – II + Physical Chemistry Practicals – II)	10	-	50	-	4
	MC12	Seminar II	-	-	25	-	1
	MC13	Viva-voce I	-	-	-	50	2
III	MC14	Chemistry of Natural Products(C)	5	3	50	50	4
	MC15	Electrochemistry and Spectroscopy(C)	5	3	50	50	4
	MC16	Medicinal Chemistry(E)	5	3	50	50	5
	MC17	Practicals III (Organic Chemistry Practicals – III + Inorganic Chemistry Practicals – III + Physical Chemistry Practicals – III)	10	-	50	-	4
	MC18	Seminar III	-	-	25	-	1
	MC19	Project-Review or Theoretical Research or Sponsored project	5	-	-	-	-
IV	MC20	Coordination Chemistry (C)	5	3	50	50	4
	MC21	Scientific Research Methodology (C)	5	3	50	50	4
	MC22	Bio-inorganic chemistry (E)	5	3	50	50	5
	MC23	Practicals IV (Organic Chemistry Practicals – IV + Inorganic Chemistry Practicals – IV + Physical Chemistry Practicals – IV)	10	-	50	-	4
	MC24	Seminar IV	-	-	25	-	1
	MC25	Comprehensive Viva voce	-	-	-	50	2
	MC19	Project-Review or Theoretical Research or Sponsored project	5	-	50	50	6
Total					1050	850	

<u>Total papers</u>	<u>Credits</u>
Theory + practicals	14 x 4 = 56
Seminars	1 x 4 = 4
Viva – voce	1 x 4 = 4
Project	6
Credits for core papers	70
Electives	4 x 5 = 20
<b>Total credits</b>	<b>90</b>

### 7. Evaluation of Project/ Review article:

#### Project Report:

	CA	50	ESE	50
Literature collection		10	Report	25
Originality/planning		5	Viva voce	25
Accuracy		10		
Comprehension		10		
Quantum of work		15		

#### Review Article

	CA	50	ESE	50
Collection of data/information		20	Report	25
Comprehension		10	Viva voce	25
Critical analysis/comparison		20		

### 8. Viva-voce:

- Viva voce - I will be held at the end of the second semester (before the ES examinations in which students will be examined in the theory and practical subjects prescribed in the first two semesters. This will be conducted by a panel of three internal examiners.

Viva voce - II (comprehensive) will be held at the end of the fourth semester (before the ES examination) in which students will be examined for over-all understanding of the various theory and practical subjects prescribed in all the four semesters. This will be conducted by a panel of three internal and three external examiners. (Students will be required to pay examination fees for viva-voce I and viva-voce II as prescribed by the Examination Office).

### 9. Community and Social Service:

- CSS programme – 30 hours.

### 10. Requirements for qualifying for M.Sc. degree in Chemistry (CBCS pattern) :

- Passing in seminar, viva-voce and project is mandatory.
- The student has to secure over all 90 credits.

## MC01: BASIC CONCEPTS IN ORGANIC CHEMISTRY

(75 hours)

### Unit I

(15 hours)

- 1.1 Aromaticity. Benzenoid and nonbenzenoid compounds. Huckel and Craig rules. Alternate and non-alternate hydrocarbons. Homo- and antiaromatic compounds.
- 1.2 Study of cyclopropenium cation, cyclopentadienyl anion, cycloheptadienyl cation. Ferrocene, Annulenes [10],[14],[18],[22]. Tropolone, Azulene.

### Unit II

(15 hours)

- 2.1 Stereochemistry: Optical activity and chirality. Classification of chiral molecules as asymmetric and dyssymmetry of allenes, biphenyls, spiro-compounds, cyclobutane and cyclononane and molecules with helical structures. Absolute configuration - R-S Notation of simple molecules including biphenyls, allenes and spiranes. Molecules with more than one asymmetric centre - erythro and threo compounds. Asymmetric synthesis, Cram's rule - optical purity.
- 2.2 Geometrical isomerism- E-Z nomenclature of olefins. Geometrical and optical isomerism of disubstituted cyclopropane, cyclobutane and cyclopentanes. Identification of enantiotropic, homotropic, diastereotropic hydrogens and prochiral carbons in compounds containing upto ten carbon atoms only. Stereospecific and stereoselective synthesis.

### Unit III

(15 hours)

- 3.1 Conformation and conformational analysis: Conformation and reactivity in acyclic systems - conformations of some simple 1,2- disubstituted ethane derivatives. Sawhorse and Newmann projections.
- 3.2 Conformation and reactivity in cyclic systems - cyclobutane, cyclopentane, cyclohexane, cycloheptane and cyclooctane. Conformational analysis of disubstituted cyclohexanes and their stereochemical features - Conformation and reactivity of cyclohexanols (oxidation and acylation), cyclohexanones (reduction) and cyclohexane carboxylic acid derivatives (esterification and hydrolysis). Conformation and stereochemistry of cis- and trans- decalins.

### Unit IV

(15 hours)

- 4.1 Study and description of organic reaction mechanisms. Non-kinetic methods. Energy profile diagrams, intermediate versus transition state, identification of products, Cross-over experiments, Stereochemical studies- uses of isotopes.
- 4.2 Kinetic methods: kinetic isotopic effects, salt effects, solvent effects- solvent isotopic effects, kinetic and thermodynamic controlled products. Hammond postulates. Curtin-Hammett principle.

### Unit V

(15 hours)

- 5.1 Structural effects: Correlation of structure with reactivity. Inductive, mesomeric, steric effects, steric inhibition of resonance, Linear free energy relationship - Hammett equation, Taft equation, acidity of carboxylic acids and phenols, basicity of aliphatic and aromatic bases.
- 5.2 Reactive intermediates: Carbocations, carbanions, carbenes, arynes, nitrenes and free radicals, anions and cations. Generation, detection, stability and reactivity.

### References:

- |   |                                   |
|---|-----------------------------------|
| 1. Advanced Organic chemistry                   | Jerry March, III Edn, McGraw Hill |
| 2. Guide book to reaction mechanism             | Peter Sykes                       |
| 3. Mechanism and structure in organic chemistry | Gould.E.S                         |
| 4. Advanced organic chemistry                   | Carey and Sundberg                |
| 5. Mechanism and theory in organic chemistry    | Lowry and Richardson              |
| 6. Stereochemistry                              | Nasipuri                          |

## MC02: MATERIALS SCIENCE

(75 hours)

### Unit I

(15 hours)

- 1.1 Structure and bonding in solids – cohesive force in crystals, van der Waal's interactions, ionic bonding, covalent bonding and hydrogen bonding in solids.
- 1.2 Structural aspects of rutile, fluorite, antiferite, zinc blende, wurtzite, cristobalite, spinels, inverse spinels and silicates.
- 1.3 Crystal geometry- symmetry elements (including glide planes and screw axis) and their operations, point groups and space groups- definition and examples.

### Unit II

(15 hours)

- 2.1 Classification of crystals- seven crystal systems and fourteen Bravais lattices;
- 2.2 Techniques of structure determination in solid state – X-ray diffraction, electron and neutron diffractions and electron microscopy – principle, instrumentation and applications; Fourier analysis in structure determination.

### Unit III

(15 hours)

- 3.1 Theories of metallic state – free electron theory, Brillouin and Band models.
- 3.2 Defects in crystals – Frenkel and Schotky defects, F-centres, effect of defects on the electrical, optical, magnetic, thermal and mechanical properties of crystals.
- 3.3 Smart metals – binary and ternary- examples and applications.

### Unit IV

(15 hours)

- 4.1 Optimised ionic conductors – silver ion, copper ion, alumina and related electrolytes, alkali metal ion, fluoride ion and proton conductors; super conductors – principle and applications.
- 4.2 Models of ionic motion – simple hopping motion cooperative motion models.
- 4.3 Photoconducting materials – principle, examples and applications.

### Unit V

(15 hours)

- 5.1 Organic semiconductors – photophysical processes, thermal and photo generation of carriers; aromatic hydrocarbons, phthalocyanines-anthracene mechanisms; excitons and polarons.
- 5.2 Charge transfer complexes – characterization and their electrical properties.
- 5.3 Conducting polymers – polyacetylenes, polyanilines and polyvinylidenes- preparation and applications.
- 5.4 Carbon nanoparticles – fullerenes –preparation and potential applications.
- 5.5 Liquid crystals – classification- thermotropic and lyotropic- nematic, smectic and cholesteric and their applications.

### References :

1. Material Science by Raghavan
2. Material Science Vol I and II by Manas Chanda
3. Structural Inorganic Chemistry A.F.Wells
4. Introduction to solid state physics McCrey et al.

## MC03: THERMODYNAMICS AND CHEMICAL KINETICS

(75 Hours)

### Unit I (15 hours)

- 1.1 Chemical Thermodynamics: Partial molal properties. fugacity and its determination. Activity and activity coefficient, determination of activity coefficients.
- 1.2 Nonequilibrium Thermodynamics : Postulates of nonequilibrium thermodynamics. Entropy production. Linear laws relative to fluxes and forces. Curie's theorem. Onsager's reciprocity relation. Relaxation phenomena.

### Unit II (15 hours)

- 2.1 Statistical Thermodynamics: Permutation and combination. Laws of probability. Distribution laws. Gaussian distribution. Microstates and macrostates for distinguishable and indistinguishable particles. Thermodynamic probability. Velocity space and phase space. MB distribution for molecular velocities. Maxwell-Boltzmann statistics. Partition functions. Use of Maxwell-Boltzmann statistics for obtaining thermodynamic quantities. Entropy and probability. Heat capacities of monoatomic gases and solids- Einstein and Debye models. Equilibrium constant calculation for isomolecular reactions. Bose-Einstein and Fermi-Dirac statistics. Classical limit. Liquid helium and BE condensation. Fermi energy. Negative absolute temperature.
- 2.2 Ensembles- calculation of thermodynamic properties.

### Unit III (15 hours)

- 3.1 Reaction Mechanisms. CTST - Potential energy surfaces, reaction coordinate. Kinetic isotope effect. Principle of microscopic reversibility-detailed balancing. Unimolecular and termolecular reactions.
- 3.2 Reactions in Solution. Comparison of gas phase reactions with reactions in solutions, factors influencing reaction rates in solution- effect of dielectric constants - primary and secondary salt effects. Application of CTST to reactions in solution, diffusion controlled reactions in solutions (cage effect).

### Unit IV (15 hours)

- 4.1 Homogeneous Catalysis. Acid base catalysis, acidity functions, Zucker-Hammett and Bunnet hypothesis. Enzyme catalysis.
- 4.2 Heterogeneous Catalysis. Physical adsorption and chemisorption- Lennard-Jones plots- adsorption isotherms- Langmuir and BET equation. Surface area measurement. Role of surface in catalysis- catalysis by semiconductor. Langmuir, Hinshelwood-Rideal and Rideal-Eley mechanisms.

### Unit V (15 hours)

- 5.1 Kinetics of Photochemical Reactions: Comparative study of thermal and photochemical mechanisms in hydrogen-halogen reactions. Decomposition of carbonyl compounds- Rice-Herzfeld mechanisms.
- 5.2 Kinetics of Polymerisation Reactions: Principle of polymerisation kinetics- molecular and free radical mechanisms.
- 5.3 Fast reactions: Methods of studying fast reactions- flow methods - relaxation technique, flash photolysis.
- 5.4 Radiolysis processes: Dosimeter- G-value- Radiolysis of water and aqueous solutions- primary and secondary processes.

### References

- |   |                          |
|---|--------------------------|
| 1. Statistical thermodynamics             | McClelland               |
| 2. Statistical thermodynamics             | Lee, Sears and Turquotte |
| 3. Elements of statistical thermodynamics | Nash                     |
| 4. Kinetics and mechanism                 | Frost and Pearson        |
| 5. Chemical kinetics                      | Laidler.                 |

## MC04: ENVIRONMENTAL CHEMISTRY

(75 Hours)

### Unit I

(15 hours)

The atmospheric chemistry - the structure of the earth's atmosphere - chemistry of the lower and upper atmospheres.

The chemistry of air pollution- - oxides of nitrogen -hydrogen sulphide and oxides of sulphur - aerosols -ozone depletion and consequences- dioxins burning plastics-other atmospheric chemicals - smog - radioactivity and fallout - air pollution abatement.

1.3 Green house effect- Global warming, oxides of carbon.

Noise pollution.

### Unit II

(15 hours)

2.1 The Lithosphere -The chemical composition of earth- the structure and composition of inner earth - the mantle - the mohorovicic discontinuity and the crust - the origin and early chemical history of the earth.

2.2 The exploitation of mineral resources and the abuse of earth -earth resources - changing the face of the land - the earth as a dump - recycle - earth resource conservation steps.

2.3 The hydrosphere: The fresh water chemistry - the structure and properties of liquid water - lakes, rivers, ponds and streams - river chemistry, pollution and aeration - water additives - isotopes - mercury pollution.

2.4 Marine chemistry- the hydration of solutes - the chemical constituents of sea water - organic matter and suspended material - ocean dumping - the estuarine and costal zone - oil pollution.

2.5 The role of water in our total environment - the hydrologic cycle - snow and ice - nucleation and precipitation - the chemical composition of rain water - phase changes and isotopic fractionation.

### Unit III

(15 hours)

3.1 The biosphere:The composition and structure of the biosphere- the biosphere as a perturbation of cosmic environment - chemical nature of the biosphere- biogenesis and the history and fate of the biomaterial - the structure of the biosphere.

3.2 The chemistry of life - fermentation and anaerobic processes - photosynthesis - respiration - decay and bio-degradation.

3.3 Man's perturbation of the biosphere - Man as a chemical factory- material use and waste - man as a chemical factory - energy use and thermal pollution - ecological disruption - chemical sensation, hormonal imbalance and mutagens - internal pollution.

3.4 Hydrosphere - lithosphere interaction: The structure of water at an interface - chemical composition of mineral water - weathering and the changing face of the land - the origin of the oceans - sedimentation and the deposition of materials from the hydrosphere - chemical exchange between sediments and the water column.

### Unit IV

(15 hours)

4.1 Lithosphere - biosphere interaction: soil chemistry - the prospects of agriculture - agricultural pollution - pesticides and other persistent pollutants - the deposition of coal and petroleum - theories of origin of petroleum .

4.2 Atmosphere - biosphere interaction and atmosphere - hydrosphere interaction: history of earth's atmosphere - the nitrogen cycle - the carbon cycle - air -sea interactions .

4.3 Biosphere - hydrosphere interaction: The chemistry of water pollution - sewage treatment, primary, secondary- and tertiary - activated sludge - trickling filters- denitrification- biology and energy chain- reactor design theory- anaerobic digestion- eutrophication.

### Unit V

(15 hours)

5.1 Pollution control in the following: Fertiliser, petroleum, pulp and paper, tanning, sugar, alcohol, electroplating and nuclear reactors.

5.2 Analysis of pollutants: Sum, specific and group parameters BOD, COD, specific oxygen demand, DOC, DOCl, DOS, Fe, Cr, Cu, Pb, and Ni - SO<sub>2</sub>, NO<sub>x</sub> H<sub>2</sub>S, O<sub>3</sub> and CO.

### References:

- |  |                                   |
|--|-----------------------------------|
| 1. Chemistry of our environment              | R.A.Horne                         |
| 2. Environmental chemistry                   | A.K.De                            |
| 3. Environmental chemical analysis           | Iain L, Marr and Malcom S.Cresser |
| 4. Pollution control in processes industries | S.P.Mahajan                       |

## **MC05: PRACTICAL I (150 HOURS)**

### **ORGANIC CHEMISTRY PRACTICAL I**

1. Separation and analysis of two component organic mixtures by chemical methods.
2. Preparations involving two stages.

### **INORGANIC CHEMISTRY PRACTICALS I**

Semimicro qualitative analysis of mixtures containing two common cations and two cations of the following less familiar elements.

Tl, W, Se, Te, Mo, Ce, Th, Ti, Zr, V, Be, U and Li.

### **PHYSICAL CHEMISTRY PRACTICALS I**

#### **I MISCELLANEOUS**

1. Heat of solution
2. Heat of neutralisation
3. Phase diagram - two components
4. Phase diagram - three components
5. Refractometry - bond refractions
6. Refractometry - interaction between the components of a binary mixture

#### **II CONDUCTOMETRY**

7. Equivalent conductance of a strong electrolyte
8. Equivalent conductance of a weak electrolyte
9. Dissociation constant of a weak acid
10. Solubility of sparingly soluble salt

## MC07: ORGANIC REACTION MECHANISM

(75 Hours)

### Unit I (15 hours)

Nucleophilic substitution at Carbon:  $S_N1$ ,  $S_N2$ ,  $S_Ni$ ,  $S_N1'$ ,  $S_N2'$  and tetrahedral mechanisms, solvolytic reactions, neighbouring group participation, ambident nucleophile, mechanisms of ester formation and ester hydrolysis.

Substitution at an aromatic centre, bimolecular mechanism, the benzyne mechanism - the unimolecular mechanism - von Richter reaction.

### Unit I (15 hours)

Elimination Reactions: E1, E2 and E1cB mechanisms, competition between elimination and substitution, orientation of product formation, stereochemistry of E2 reactions, intramolecular pyrolytic eliminations, the Chugaev reaction, Cope elimination.

Addition reactions: Electrophilic addition to alkenes, kinetics, effect of structure, isotope effects, orientation and stereochemistry, the nature of the intermediates, ozonolysis, hydroboration, additions to dienes, alkynes (halogenation and hydrogenation) and allenes, Diels-Alder reaction, 1,3 dipolar additions.

Nucleophilic addition to multiple bonds, Mannich reactions-Aldol and related reactions, Stobbe, Cannizzaro reaction, Darzens, Thorpe and Wittig reaction, benzoin condensation Cram's rule.

### Unit III (15 hours)

Electrophilic substitution: The  $S_E1$ ,  $S_E2$  and  $S_Ei$  mechanisms, electrophilic substitution via enolization, Stork-enamine reaction. Electrophilic displacements at an aromatic carbon, the general mechanism, kinetics of  $S_E2$ -Ar reactions, the kinetic isotope effects, structural effects on rates, the ortho-para selectivity ratio, Vilsmeier formylation, Gatterman-Koch reaction, Jacobson reaction.

Oxidation and reduction reactions: Oxidation of alcohols using chromic acid- DMSO-DCC- hydroxylation of olefins (both cis and trans), cleavage of 1,2-glycols using periodate, lead tetra acetate- oxidation using  $SeO_2$ . Catalytic hydrogenation, metal hydride reduction, Birch reduction.

### Unit IV (15 hours)

Pericyclic reactions: Application of HMO theory to organic reaction mechanisms. Electrocyclic (butadiene-cyclobutene system), cyclo-addition ((4 +2) and (2+2)) systems, sigmatropic and cheletropic reactions, use of FMO and correlation diagrams.

Organic photochemistry: General principles- photochemistry of carbonyl compounds- Norrish Type I and Type II reactions. Photoreduction, Paterno-Buchi- di-pi-methane rearrangement, Barton rearrangement.

### Unit V (15 hours)

Molecular rearrangements: Wagner-Meerwein, Pinacol and related rearrangements, Demjanov, dienone-phenol rearrangements, Baeyer-Villiger oxidation, Beckmann, Schmidt, Wolff, Stevens, Sommelet-Hauser, Wittig, Benzil-benzilic acid, Favorskii, benzidine rearrangements.

Reagents in organic synthesis and functional groups transformation-complex metal hydrides, lithium dimethylcuprates, lithium di-isopropylamide (LDA), 1,3 dithiane and trimethylsilyliodide.

### References:

1. Advanced organic chemistry Jerry March. 4th ed..McGraw-Hill
2. Guide book to reaction mechanisms Peter Sykes
3. Mechanism and structure in organic chemistry E.S.Gould.
4. Advanced Organic Chemistry Carey and Sundberg, Parts A & B.
5. Mechanism and theory in Organic Chemistry Lowry and Richardson

**MC08: ANALYTICAL TECHNIQUES IN CHEMISTRY**  
(75 Hours)

Unit I (15 hours)

Electronics: Basic functions of instrumentation - semiconductor components - operational amplifiers - signal to noise ratio - sources of noise - Instrument calibration.

Thermal methods: Thermogravimetric and differential thermal analysis, thermometric titrations, differential scanning calorimetry - basic instrumentation and applications.

Chromatographic methods: TLC, column, gas, ion exchange and gel - permeation chromatography - principles and applications.

Unit II (15 hours)

Nuclear magnetic resonance - principle, instrumentation, structure determination.

Electron spin resonance - principle, instrumentation and interpretation of esr spectra application to coordination compounds.

Mass spectrometry - principle, basic instrumentation - fragmentation patterns - organic molecular structural determination - applications in the study of inorganic compounds.

Unit III (15 hours)

Optical methods of analysis: Colorimetric analysis and uv- visible spectroscopy: The importance and applications of Beer-Lambert's law. uv - visible spectrophotometric analysis - principles - single and double beam instruments - basic instrumentation - determination of Fe, Co, Mn and Ti - analysis of organic compounds - olefins, ketones and aromatics by uv- visible spectroscopy (Woodward - Fieser rules).

Infrared spectrophotometric analysis - principle - instrumentation - molecular structure determination.

Raman spectra - principle, basic instrumentation - diagnostic structural analysis.

Unit IV (15 hours)

Flame photometric and atomic absorption analysis - atomic fluorescence - principles and applications.

ORD and circular dichroism - Cotton effect - axial halo-ketone rule - Octant rule - applications.

5. Mössbauer spectroscopy - principle, instrumentation-applications.

Unit V (15 hours)

Electroanalytical methods: polarography - principle, instrumentation and applications. Derivative polarography- Cyclic Voltametry - principle.

Amperometric titration - principle and examples.

Radiochemical methods: hot atom chemistry - The Szilard-Chalmers process, chemistry of recoil atoms, chemical effects of radioactive decay, solvated electron.

Uses of radiations in the study of matter, neutron activation analysis, dilution analysis, dosimetry, synthesis of organic and inorganic compounds by irradiation radiometric analysis, radiography.

References:

- |   |                                   |
|---|-----------------------------------|
| 1. Fundamentals of analytical chemistry | Skoog and West                    |
| 2. Quantitative chemical analysis       | Saunders and Toppan               |
| 3. Instrumental methods of analysis     | Willard, Merritt, Dean and Settle |
| 4. Analytical chemistry                 | G.Dick                            |

## MC09: GROUP THEORY AND QUANTUM MECHANICS

(75 hours)

### Unit I (15 hours)

- 1.1 Fundamentals of group theory.
- 1.2 Symmetry-elements and operations in molecules; point groups; matrix representations.
- 1.3 Character tables- formation and use of character tables in predicting hybridisation and IR, Raman active vibrations.

### Unit II (15 hours)

- 2.1 Application of group theory- to electronic spectra of ethylene and formaldehyde, benzene and butadiene.
- 2.2 Introduction to quantum mechanics-general principles of classical mechanics and its failure; postulates of quantum mechanics;
- 2.3 Functions and operators - eigenfunctions, eigenvalues, Hamiltonian operator, angular momentum operators - commutation of operators.

### Unit III (15 hours)

- 3.1 Application of Quantum Mechanics-particle in a box, simple harmonic oscillator - rigid rotor, hydrogen atom; - atomic units.
- 3.2 Approximation Methods-variation method and perturbation method (time- independent) - simple examples.

### Unit IV (15 hours)

- 4.1 HMO Calculations-evaluation of coefficients and eigen values for simple molecules; electron density-bond order and free valence index.
- 4.2 Symmetry adapted linear combination-application to benzene and naphthalene.
- 4.3 Extended HMO theory-application to simple ring molecules containing hetero atoms.

### Unit V (15 hours)

- 5.1 Many electron atoms- Helium atom; general principle of setting up wave function for other many - electron atoms - Pauli principle.
- 5.2 Slater type orbitals - Hartree and Hartree-Fock SCF methods; Born-Oppenheimer approximation.
- 5.3 Bonding- VB and MO treatment of  $H_2$  and  $H_2^+$  - MO theory for homonuclear and heteronuclear diatomic molecules.
- 5.4 Hybridisation involving s, p, d orbitals - use of hybrid orbitals in constructing MO models of  $N_2$ ,  $O_2$  and CO.

### References:

- |                                      |                  |
|--------------------------------------|------------------|
| 1. Application of group Theory       | F.A.Cotton       |
| 2. Programmed text for group theory  | Allen Vincent    |
| 3. Group theory                      | Bishop           |
| 4. Symmetry in chemistry             | Jaffe and Orchin |
| 5. Introduction to quantum chemistry | A.K.Cotton       |
| 6. Quantum chemistry                 | D. A. Mc Quarrie |
| 7. Quantum mechanics                 | Hanna            |
| 8. Quantum chemistry                 | Levine           |
| 9. Quantum chemistry                 | La Paglia        |
| 10. Quantum mechanics                | Anantharaman     |

## MC10: POLYMER CHEMISTRY

(75 hours)

### Unit I: (15 hours)

- 1.1 Basic concepts of polymer chemistry: Repeat unit, degree of polymerisation, classification, stereochemistry of polymers, nomenclature of stereoregular polymers.
- 1.2 Chain polymerisation, free radical polymerisation, ionic polymerisation and coordination polymerisation: Zeigler- Natta catalyst, step polymerisation, ring opening polymerisation.
- 1.3 Copolymerisation: Block and graft copolymers - preparation.

### Unit II: (15 hours)

- 2.1 Polymerisation techniques: Bulk, solution, suspension, emulsion, polymerisations; Melt polycondensation, solution polycondensation, interfacial condensation, solid and gas phase polymerisation.
- 2.2 Molecular weight and size: Number average and weight average molecular weights, polydispersity and molecular weight distribution in polymers, the practical significance of polymer molecular weights and size of polymers.
- 2.3 Glass transition temperature: Concept of glass transition temperature and associated properties, glassy solids and glass transition, factors influencing glass transition temperature.
- 2.4 Crystallinity in polymers: Polymer crystallisation, structural and other factors affecting crystallisability, effect of crystallinity on the properties of polymers.

### Unit III: (15 hours)

- 3.1 Processing: Calendering, die casting, rotational casting, film casting, compression moulding, injection moulding, blow moulding, extrusion moulding, thermoforming, foaming and reinforcing techniques.
- 3.2 Synthetic resins and plastics: Manufacture and applications of polyethylene, PVC, teflon, polystyrene, polymethylmethacrylate, polyurethane, phenol-formaldehyde resins, urea-formaldehyde and melamine-formaldehyde resins and epoxy polymers.

### Unit IV: (15 hours)

- 4.1 Synthetic fiber's: Rayon, nylons, polyesters, acrylics, modacrylics, spinning techniques.
- 4.2 Natural rubber: Production, constitution, vulcanization (hot and cold), fillers and accelerators, antioxidants.
- 4.3 Synthetic rubber: SBR, butyl rubber, nitrile rubber, neoprene, silicone rubber and polysulphides.

### Unit V: (15 hours)

- 5.1 Polymer degradation: Types of degradation- thermal, mechanical, photo, hydrolytic and oxidative degradations.
- 5.2 Additives for polymers: Fillers, plasticisers, thermal stabilizers, photo stabilizers, antioxidants and colourants.

#### References:

1. Text book of polymer science Billmeyer
2. Polymer science Gowariker et al.
3. First course in polymer chemistry Strepikheye et al.

## MC11: PRACTICALS – II (150 HOURS)

### ORGANIC CHEMISTRY PRACTICAL II

1. Separation and analysis of two and three component organic mixtures by chemical methods.
2. Preparations involving three stages.

### INORGANIC CHEMISTRY PRACTICAL II

1. Colorimetric estimations using Nessler's technique and colorimeter: Cu, Fe, Ni and Mn.
2. About twelve preparations involving different techniques.

### PHYSICAL CHEMISTRY PRACTICAL II

#### I Miscellaneous

1. Freundlich adsorption isotherm
2. Beer - Lambert's law - simultaneous estimation of Mn and Cr in a solution containing  $\text{KMnO}_4$  and  $\text{K}_2\text{Cr}_2\text{O}_7$ .
3. Molecular weight determination by the Beckmann method

#### II Conductometric Titrations

4. HCl vs NaOH
5. HCl and  $\text{CH}_3\text{COOH}$  vs NaOH
6.  $\text{Cl}^-$  and  $\text{I}^-$  vs  $\text{AgNO}_3$
7.  $\text{CuSO}_4$  vs NaOH or  $\text{MgSO}_4$  vs  $\text{BaCl}_2$

#### III EMF Measurements

8. Standard Electrode Potential
9. Solubility of AgCl or AgBr
10. pH of buffer
11.  $\text{pK}_a$  of weak acid
12. Determination of  $\text{K}_h$  of a weak salt

## MC14: CHEMISTRY OF NATURAL PRODUCTS

(75 Hours)

### Unit I (15 hours)

- 1.1 Heterocyclic compounds, synthesis and reactions of imidazoles, oxazoles, thiazoles, pyridazines, pyrimidines and pyrazines.
- 1.2 Natural pigments: Anthocyanins - general methods of determining structure and synthesis - cyanin and hirsutin chlorides. Flavones and Flavanols - general method of determining structure and synthesis - Quercetin- Isoflavones - daidzein.
- 1.3 Carbohydrates: Structural aspects of starch and cellulose.

### Unit II (15 hours)

- 2.1 Terpenes: classification, structural elucidation by chemical degradation and synthesis of  $\alpha$ -pinene, camphor, zingiberene, santonin,  $\beta$ -carotene.
- 2.2 Steroids: Structure and synthetic aspects of cholesterol, ergosterol, estrone and progesterone.

### Unit III (15 hours)

- 3.1 Alkaloids: classification, structural elucidation by chemical degradation and synthesis of papaverine, quinine, morphine and reserpine.
- 3.2 Antibiotics: structure and synthesis of chloramphenicol, penicillins and streptomycin.

### Unit IV (15 hours)

- 4.1 Vitamins: Structure and synthesis of vitamin A, B<sub>1</sub>, B<sub>2</sub>, B<sub>6</sub>, C, D, E, K and H.
- 4.2 Proteins: structural aspects of protein, DNA and RNA. Enzymes - classification, structure and mode of action.

### Unit V (15 hours)

- 5.1 Synthetic methodology: protection of functional groups (hydroxyl, amino, carboxyl, and carbonyl-groups), Illustration of protection and deprotection in synthesis - synthetic analysis and planning- synthesis of target molecules based on disconnection and synthon approach. Control of stereochemistry- synthesis using simple chiral molecules.
- 5.2 Biosynthesis: Biosynthetic routes for terpenes, alkaloids, steroids, carbohydrates, proteins and insulin.

### References:

- |                                      |                 |
|--------------------------------------|-----------------|
| 1. Organic chemistry                 | I.L.Finar vol 2 |
| 2. Oxidation reduction               | Reinhardt       |
| 3. Heterocyclic chemistry            | Joule and Smith |
| 4. Biosynthesis of organic compounds | Bu'lock         |

## MC15: ELECTROCHEMISTRY AND SPECTROSCOPY

(75 Hours)

### Unit I

(15 hours)

- 1.1 Ion-solvent interaction: Born's treatment of ion solvent interaction - its validity and modification. A brief account of the ion-dipole and ion-quadrupole models of ion-solvent interactions.
- 1.2 Ion-Ion interactions and activity coefficients: Debye - Huckel ionic atmosphere model of the strong electrolytes - derivation of Debye - Huckel limiting law - validity of the equation- extension of Debye - Huckel equation - Significance of the activity coefficient of electrolytes.
- 1.3 Ion-transport in solutions: Theory of strong electrolytes for electrolytic conduction- Debye Huckel ion atmosphere model - Derivation of the Onsager equation - validity of the equation - modification of the Onsager equation.
- 1.4 Ion Association: Bjerrum treatment of association - Bjerrum ion association constant - factors influencing ion-association - effect of ion- association on conductivity and activity coefficient of electrolytes in solution.

### Unit II

(15 hours)

- 2.1 Dynamic electrochemistry: The electrified interface - IHP, OHP, contact adsorption - surface excess and its importance - use of mercury in double layer studies.
- 2.2 Thermodynamics of electrified interfaces- Electrocapillary measurements - Lipmann potential - polarisable and non-polarisable interfaces - Billiter potential.
- 2.3 Structure of electrified interfaces- Discussion of various models - Helmholtz- Perrin, Gouy-Chapmann and Stern Models - derivations of equations and their validity. electrokinetic phenomena - Electrokinetic effects -concepts and derivations of equations - Zeta potential and its determination- Tsilius method of separation of proteins - stability of colloids.
- 2.4 Electrodeics: Charge transfer across the electrified interface - its chemical and electrical implications - the basic electrodic equation- the Butler - Volmer equation- derivation and its significance-special cases of Butler-Volmer equation. Concept of overpotential - types of overpotential - quantification of polarisable and non-polarisable interfaces.
- 2.5 A brief account of hydrogen overpotential- factors influencing the hydrogen overpotential and the mechanism. Concentration polarisation and its application- expression for limiting current density - current-potential curves. Basis of polarography - application of polarographic technique.
- 2.6 Power generation : Fuel cells - construction and principle of operations and applications. Photovoltaic phenomenon in electrochemical cells.
- 2.7 Corrosion: Theory of corrosion - techniques for inhibiting corrosion.

### Unit III

(15 hours)

- 3.1 Atomic spectra: Total angular momentum vector- spectral notations - term symbols - selection rules - spectra of one and two electron systems- effect of magnetic and electric fields - Zeeman and Stark effects.
- 3.2 Electronic spectroscopy: Electronic spectra of diatomic molecules - Frank Condon Principle. Dissociation and predissociation - simple chromophores - Fluorescence and phosphorescence. Electronic spectrum of polyatomic molecules- conjugated system.
- 3.3 Photoelectron spectroscopy: Origin - chemical shift - MO's - spectra involving core and valence electrons applications.

#### Unit IV

(15 hours)

- 4.1 Pure rotational spectra: Quantum mechanical results on the rigid rotor. Rotational constant - centrifugal distortion . Classification of molecules according to their moment of inertia - Stark effect - inversion - spectrum of ammonia - Rotational Raman spectra - anisotropic polarizability. Stokes and antistokes lines .
- 4.2 Vibrational - spectra - Harmonic oscillator - diatomic molecules, force constants, Fundamental vibration frequencies- Anharmonicity of molecular vibrations and its effect on vibrational frequencies - second and higher harmonics.
- 4.3 Vibration - rotation spectra, P,Q and R branches- vibrational Raman spectra of diatomic molecules - vibrations of polyatomic molecules-normal modes of vibrations - CO<sub>2</sub>, H<sub>2</sub>O and acetylene.

#### Unit V

(15 hours)

- 5.1 Nuclear magnetic resonance spectra: Theory - the nuclear spin - Larmor frequency, NMR isotopes, population of nuclear spin levels - relaxation processes. Chemical shift shielding constant - ring currents and aromaticity - shifts for <sup>1</sup>H and <sup>13</sup>C . - spin-spin interaction - low and high resolution spectra. Nuclear magnetic double resonance - nuclear overhauser effect. <sup>13</sup>C-NMR. Applications to structure elucidation of simple organic molecules. FT NMR- principle. Electron spin resonance spectra. Theory - hyperfine splitting - energy levels for a radical with a single set of equivalent protons and multiple sets of equivalent protons.
- 5.3 Mössbauer spectroscopy. Principle, chemical isomer shift, quadrupole splitting, Zeeman splitting - applications .

#### References:

- |                                  |                                       |
|----------------------------------|---------------------------------------|
| 1. Modern electrochemistry       | Bockris and Reddy Vols. I & II        |
| 2. Electrochemistry              | Glasstone                             |
| 3. Molecular spectroscopy        | Barrow                                |
| 4. Molecular spectroscopy        | Chang                                 |
| 5. Spectroscopy                  | Straughan and Walker Vols.I.,II & III |
| 6. Molecular spectroscopy        | Graybeal                              |
| 7. Physical methods in chemistry | Drago                                 |

**MC 16: MEDICINAL CHEMISTRY**  
(60 hours)

Unit.I (12 hours)

- 1.1 Interdisciplinary nature of medicinal chemistry – Pharmacology, Molecular Pharmacology, Microbiology, Biochemistry, Physiology, Medicine and Pharmacy.
- 1.2 Classification of Drugs – Central Nervous system acting drugs- (General and Local anaesthetics, Sedatives and Hypnotics, Anticonvulsants, Narcotic and Non-narcotic analgesics, Anti-Parkinsonian agents, Anti-depressants, Tranquilizers, Psychomimetics), Pharmacodynamic agents (Anti-arrhythmics, Anti-anginals, Vasodilators, Anti-hypertensives, Diuretics, Antihistamines), Chemotherapeutic Agents (Antibiotics, Antivirals, Antifungals), Drugs for metabolic and endocrine disorders (Anti-thyroid drugs, Antidiabetic drugs, biosynthetic insulin), Therapeutic Index. (Definitions with examples).
- 1.3 Pharmaceutical Phase – Routes of administration (gastrointestinal, lungs, parenteral), Dosage forms – ingredients, their role, and manufacture (tablets, capsules, liquids, injectables, suppositories, creams and pastes). Slow release drug formulations.

Unit.II (12 hours)

- 2.1 Pharmacokinetic Phase- Structure of eucaryotic cell (Cell components and their functions, Cell membrane models, Passive and Active transport of materials across cell membranes, Pinocytosis)
- 2.2 Drug action and physicochemical properties - hydrophobicity, electronic effect, steric effect.
- 2.3 Quantitative Structure Activity Relationships (QSAR Studies ) – Hansch Equation, The Craig Plot, The Topliss decision tree approach, Bio-isosterism.
- 2.4 Pharmacodynamic Phase- Drug action at receptors (the concept of receptors, structurally specific and structurally non-specific drugs, radiochemical studies of receptor sites, Agonists and Antagonists, binding force between drug and receptors).
- 2.5 Drug - receptor theories : Occupancy theory, Rate theory, Induced fit theory, Activation-aggregation theory.

Unit III (12 hours)

- 3.1 Mechanism of drug action at enzymes – competitive (reversible) inhibitors, non-competitive (irreversible) inhibitors, non-competitive reversible (allosteric) inhibitors.
- 3.2 Use of 5-fluorouracil as a transition-state inhibitor.
- 3.3 Mechanism of transamination reaction and its inhibition.
- 3.4 Mechanism of action of penicillins and cephalosporins.
- 3.5 Mechanism of insecticidal action of organophosphorous compounds.
- 3.6 Mechanism of action of allopurinol in the treatment of gout.
- 3.7 Mechanism of drugs acting on DNA – intercalating agent (proflavin), alkylating agents (uracil mustard and cis platin), chain cutting agents (bleomycin).

#### Unit.IV

(12 hours)

- 4.1 The Nervous system- Structure of nerve cells, Blood-brain barrier, The synapse, Neuro-transmitters ( acetyl choline,adrenaline), Central nervous system neuro-transmitters.
- 4.2 Drug Metabolism - Routes of elimination(kidney,biliary excretion), factors affecting drug metabolism.
- 4.3 Metabolic Processes - Phase I Reactions (oxidation, reduction, hydrolysis), Phase II Reactions - Glucuronide conjugation, acylation, methylation, mercapturic acid formation, sulphate conjugation.

#### Unit V

(12 hours)

- 5.1 Synthesis of the following drugs and their chemical uses:  
(i) Procaine hydrochloride, (ii) Meprobamate, (iii) Oxy-phenbutazone, (iv) Hydralazine hydrochloride, (v) Methyl dopa, (vi) Propranolol hydrochloride, (vii) Isopropamide iodide, (viii) Chlorpheniramine maleate, (ix) Indomethacin, and (x) Ibuprofen.
- 5.2 Principles of quantitative analysis of the following drugs in formulations:  
(i) Aspirin, (ii) Benzylpenicillin, (iii) Ascorbic acid, (iv) Dapsone, (v) Isoniazid (vi) Codeine, (vii) Chloramphenical, (viii) Riboflavin, (ix) Adrenaline, and (x) Folic acid.

#### References:

1. Introductory medicinal chemistry, J.B. Taylor and P.D. Kenewell
2. Principles of medicinal chemistry, Lea and Febiger
3. An introduction to medicinal chemistry, G.L. Patrick
- Essentials of medicinal chemistry, Korolkoras and Burckhalter
- Practical pharmaceutical chemistry, Beckett and Stenlake (vol 1 and 2)
- Quantitative analysis of drugs, D.C. Garratt
- Text book of organic medicinal and pharmaceutical chemistry, Wilson, Gisvold and Doerge
- Jenkin's quantitative pharmaceutical chemistry, A.M. Knevel and F.E. Digangi

## MC17: PRACTICALS III (150 HOURS)

### ORGANIC CHEMISTRY PRACTICALS III

1. Estimation of
  - i. Phenol
  - ii. Aniline
  - iii. Methyl ketone
  - iv. Glucose
  - v. Acetyl group
  - vi. Methoxy group
  - vii. Degree of unsaturation
  - viii. Amines and
  - ix. Nitro group
2. Characterisation of individual compounds by spectroscopic methods.

### INORGANIC CHEMISTRY PRACTICALS III

- I. Titrimetry :
  - a. Redox titrations using ceric salts. Estimation of i. iron ii. nitrite.
  - b. complexometric titrations involving the estimations of i. Ca ii Mg, iii. Ni iv. Zn and v. hardness of water.
- II. Quantitative separation and analysis (one by volumetric and one by gravimetric method) of the following artificial mixtures:
  - i. Cu and Ni ii. Cu and Fe and iii. Fe and Ni. iv. Zn and Cu.

### PHYSICAL CHEMISTRY PRACTICALS III

#### I Miscellaneous

Job's continuous variation method  
CMC determination by conductance method  
Ultrasonic interferometry

#### II Kinetics

- 4 Hydrolysis of methyl ethanoate - comparison of acid strength
- 5 Hydrolysis of methyl ethanoate -  $E_a$  determination
- 6 Effect of  $\mu$  on persulphate - iodide reaction
- 7 Iodination of acetone
- 8 Guggenheim's method

#### III Potentiometric Titrations

- 9 HCl vs NaOH
- 10 HCl and  $\text{CH}_3\text{COOH}$  vs NaOH
- 11  $\text{Cl}^-$  and  $\text{I}^-$  vs  $\text{AgNO}_3$
- 12  $\text{Fe}^{2+}$  vs  $\text{K}_2\text{Cr}_2\text{O}_7$

## MC20: COORDINATION CHEMISTRY

(75 Hours)

### Unit I (15 hours)

- 1.1 Review of the fundamentals of coordination chemistry: Distinction between double salts and coordination compounds-nomenclature-isomerism-types of ligands- common coordination numbers and geometries- 18 electron rule- stable, unstable, inert and labile complexes - methods of preparation of complexes - detection of complex formation - applications of complexes in analysis and metallurgy.
  - 1.2 Theories of bonding in complexes: Crystal field theory - splitting of d orbitals in octahedral, tetrahedral and square planar symmetries - measurement of  $10Dq$  - factors affecting  $10Dq$  - crystal field stabilisation energy - evidences for crystal field splitting - octahedral vs tetrahedral and octahedral vs square planar coordinations - site selections in spinels and antispinel - Jahn Teller distortions and its consequences. Ligand Field Theory and Molecular Orbital Theory-Group theoretical treatment of the sigma and pi bonding in complexes.
- Stability of complexes. Thermodynamic stability - stepwise and overall stability constants - their relationships - factors affecting the stability of complexes - chelate effect - importance of chelates - determination of stability constants of complexes (spectrophotometric, polarographic and pH solubility and ion exchange methods).

### Unit II (15 hours)

- 2.1 Spectral and magnetic characteristics of complexes: Term states for d ions - characteristics of d-d transitions - charge transfer spectra - selection rules for electronic spectra - Orgel correlation diagrams - Sugano-Tanabe energy level diagrams - spectrochemical series - nephelauxetic series - spin-orbit coupling - effect of spin-orbit coupling on magnetic moments - quenching of orbital magnetic moments - applications of IR, Raman and ESR, NMR, Mossbauer, ORD to the study of coordination compounds.

### Unit III (15 hours)

- 3.1 Kinetics and mechanisms of reactions of complexes: Substitution reactions of octahedral complexes - mechanism of water replacement - acid hydrolysis of octahedral complexes - base hydrolysis -  $S_NCB$  mechanism.
- 3.2 General mechanism of square planar substitution reactions - two parallel pathways - factors affecting the reactivity of square planar complexes of  $d^8$  metal ions - trans effect - theories of trans effect.
- 3.3 Mechanism of electron transfer reactions - outer sphere electron transfer reactions - Marcus-Hush theory - inner sphere electron transfer reactions - formation and rearrangement - nature of the bridge ligand in inner sphere electron transfer reactions - noncomplementary reactions. Photochemical reactions of transition metal complexes - photosubstitution - photoisomerisation - photoredox - and solar energy conversion.

### Unit IV (15 hours)

- 4.1 The complexes of alkali and alkaline earth metals with macrocyclic ligands, crown ethers - cryptands.
- 4.2 Organometallic compounds of transition elements: 16 and 18 electron rule and organometallics. Synthesis reactions, bonding and structure of metal-olefin, metal-acetylene, metal-allyl and metal-cyclopentadienyl complexes of transition elements. Oxidative addition, reductive elimination, insertion, alpha.beta elimination reactions. Fluxional isomerism of organometallics.
- 4.3 Industrial applications of organometallics as catalysts: Homogeneous and heterogeneous catalytic reactions - hydrogenation of olefins (Wilkinson's catalyst) - hydroformylation of olefins using cobalt or rhodium catalysts (oxoprocess) - olefin isomerisation - water gas shift reaction - oxidation of olefin (Wacker process) - cyclo-oligomerisation of acetylenes using Reppe's catalysts - polymerisation of olefins (Zeigler-Natta catalyst) - Fischer-Tropsch process - polymer supported catalysts.

## Unit V

(15 hours)

- 5.1 Stabilisation of the unusual oxidation states of metals. Metal carbonyls - nitrosyls - carbonyl halides - carbonyl hydrides - synthesis, bonding and structure - complexes with substituted phosphine and arsine ligands - cyano complexes - complexes with oxygen and fluorine ligands. Carbonyl clusters.
- 5.2 Bioinorganic Chemistry: Metalloporphyrins - chlorophyll - cytochromes - haemoglobin, myoglobin - synthetic oxygen carriers - vitamin B<sub>12</sub> -enzymes(structure and function) - iron sulphur proteins - biological systems - molecular nitrogen and molecular oxygen complexes.

### References:

- |   |                                 |
|---|---------------------------------|
| 1. Inorganic chemistry                    | Huheey, 4 <sup>th</sup> Edition |
| 2. Coordination chemistry                 | Basolo and Johnson              |
| 3. Organometallic chemistry               | Parkins and Poller              |
| 4. Mechanisms of inorganic reactions      | Basolo and Pearson              |
| 5. Valency and molecular structure        | Cartmell and Fowles             |
| 6. Principles of organometallic chemistry | G.E.Coates et al                |
| 7. Modern aspects of inorganic chemistry  | Emeleus and sharpe              |
| 8. Inorganic Chemistry                    | Purcell and Kotz                |
| 9. Inorganic Chemistry                    | Porterfield                     |
| 10. Concise Coordination Chemistry        | R.Gopalan and V.Ramalingam      |
| 11. Theoretical Inorganic Chemistry       | Day and Selvin                  |
| 12. Modern Inorganic Chemistry            | W.L.Jolly                       |
| 13. Introduction to ligand Fields         | Figgis                          |

## MC21: SCIENTIFIC RESEARCH METHODOLOGY

(60 Hours)

### Unit I (12 hours)

- 1.1 Chemistry literature survey-types of Chemistry literature- Primary, secondary and tertiary-examples.
- 1.2 Journals published by the ACS and RSC- CA and its importance - Indian Journals - Reviews, monographs data books and indexes.
- 1.3 Literature survey: Methods of searching literature, methods of compilation and preservation and retrieval of collected literature.
- 1.4 Research experiments: Planning and conducting experiments, methodology of collecting scientific data (with three types of project titles as examples)

### Unit II (12 hours)

- 2.1 Project report writing: The general format, chapter format, page format.
- 2.2 Procedure for presenting tables, graphs and figures; foot-notes, bibliography, appendices.
- 2.3 Abbreviations, symbols, SI units, nomenclature
- 2.4 Scientific exactness and proper language, editing.

### Unit III (12 hours)

- 3.1 Entrepreneurship: Steps in establishing a chemical factory.
- 3.2 Methodology of market survey for chemicals and chemical-based products.
- 3.3 Principles of designing bench scale production and scaling up for a chemical production computer aided analysis and computer programming.
- 3.4 Computer hardwares and softwares, implementation, software vs hardware, data representation, computerised instrumentation systems, microcomputer interfacing, computer controlled laboratory automation systems.

### Unit IV (12 hours)

Simple programs in the C language- formulation of algorithm, flowcharts, constants and variables, data types, operations and symbols, arithmetic expressions, common mathematical functions, input and output, making decisions, program looping arrays, functions, structures, character strings, pointers.

### Unit V (12 hours)

Statistical Calculation: Presentation of data, measures of central tendency, mean, standard deviation, measures of variability, simple sampling techniques, errors in chemical analysis, linear regression and correlation, method of least squares.

### References:

1. Thesis and assignment writing Anderson, Durtson and Poole
2. Handbook for authors in the Journal of the American Chemical Society Publications .
3. Chemical publications - Their nature and uses M.G.Mellon
4. Organic chemistry Jerry March, 4<sup>th</sup> edition., McGraw-Hill
5. Text book of practical organic chemistry Vogel
6. Text book of practical inorganic chemistry Vogel
7. The C language Curningham and Ritchie
8. The spirit of C Cooper
9. Understandine C Bruce H.Hunter
10. Programming in the C language Byron S.Gotfried
11. Programming in C Stephen G. Kochan
12. Modern elementary statistics John E. Freund
13. Statistical methods S.P.Gupta.
14. Principles of industrial chemistry Chris Clatesen and Guy Martisen.

## MC 22: BIOINORGANIC CHEMISTRY

(60 hours)

### Unit I

(12 hours)

Metal storage transport and biomineralisation: Ferritin, transferrin and siderophores – ion transport in membranes, membrane potential, Na, K balance, trace metals, micronutrients.

### Unit II

(12 hours)

Calcium in biology: Calcium in living cells, transport and regulation, molecular aspects of intramolecular processes, extracellular binding proteins.

### Unit III

(12 hours)

Metalloenzymes: Zinc enzymes – carboxy peptidase and carbonic anhydrase, catalase, peroxidase. Copper enzymes – superoxide dismutase, molybdenum oxatransferase enzymes – xanthine oxidase

### Unit IV

(12 hours)

Metal nucleic acid interactions: metal ions and metal complex interactions, metal complexes – nucleic acids.

### Unit V

(12 hours)

Metal in medicine: metal deficiency and diseases, toxic effect of metals, metals used for diagnosis and chemotherapy with particular reference to anticancer drugs.

### Reference:

1. Principles of bioinorganic chemistry, S.J. Lippard and J.M. Berg, University science books
2. Inorganic biochemistry, vols. I and II, ed. G.L. Eichhorn, Elsevier publications.
3. Progress in inorganic chemistry, vols. 18 and 38, ed. J.H.J. Lippard, Wiley publications.

## MC23 : PRACTICAL IV (150 HOURS)

### ORGANIC CHEMISTRY PRACTICAL IV

1. Separation using chromatographic methods
  - i) plant pigments by column
  - ii) mixture of dyes by TLC
  - iii) mixture of amino acids by paper
2. Soxhlet extraction - demonstration
3. Analysis of oils - iodine value- saponification value
4. Analysis of Vitamin C tablets and fruit juices
5. Isolations:
  - i. Caffeine from tea leaves
  - ii. Casein from milk
  - iii. Nicotine from tobacco
  - iv. Red pigment from red chillies
  - v. Cholesterol from egg.

### INORGANIC CHEMISTRY PRACTICAL IV

- I. Analysis of any two of the following alloys:
  - a. brass
  - b. bronze
  - c. solder
  - d. stainless steel
- II Analysis of any two of the following minerals
  - a. dolomite
  - b. pyrolusite
  - c. zinc blende
  - d. chrome-iron ore.
- III Separation techniques – column, paper, thin layer and ion-exchange chromatography.
- IV. Preparation and characterisation of any two complexes.  
Polarographic estimation of Cd

### PHYSICAL CHEMISTRY PRACTICAL IV

- I Kinetics:  
Hydrolysis of ethyl ethanoate by NaOH - conductance method  
Polarimetry - comparison of acid strengths  
Oxidation of alcohols by acidified  $K_2Cr_2O_7$
- II Miscellaneous:
  4. Flame Photometry
  5. Electrogravimetry - Separation of Cu and Ni
  6. Determination of  $\Delta G$ ,  $\Delta H$  and  $\Delta S$  by emf method
  7. Determination of dielectric constant of a solvent
  8. Determination of dipole moment
- III Polarography:
  9.  $E_{1/2}$  determination
  10. Concentration of an ion
  11. Stability constant of a complex