

JECRCTM
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Department of Chemistry
Course Structure and Syllabi
M.Sc. Course
(Chemistry)

Session 2020-21

JECRC University, Jaipur

Department of Chemistry

M. Sc. Syllabus

(Session 2020-2021)

SEMESTER WISE STRUCTURE OF THE M.Sc. (CHEMISTRY) PROGRAMME SEMESTER – I

Old Code	New Code	Title of Course	Credits
MCE 001C	MCE 001D	Compounds of Different Elements	4
MCE 002B	MCE 002B	Reaction Mechanism : Structure and Reactivity	4
MCE 003B	MCE 003C	Quantum, Surface and Electro Chemistry	4
MCE 004B	MCE 004B	Methamatics and Computers for Chemists	4
MCE 005A	MCE 005A	Qualitative and Quantitative Analysis (Practical)	12
			Total Credits = 28

SEMESTER – II

Old Code	New Code	Title of Course	Credits
MCE 007B	MCE 007B	Chemistry of Transition Metals	4
MCE 008A	MCE 008A	Reaction Mechanism : Addition, Elimination and Pericyclic Reactions	4
MCE 009B	MCE 009C	Thermo Dynamics and Chemical Kinetics	4
MCE 010B	MCE 010C	Applications of Spectroscopy	4
MCE 011A	MCE 011A	Chromatographic Seprations, Organic Synthesis and Potentiometric Analysis (Practical)	12
			Total Credits = 28

SEMESTER – III

Paper MCE 013A is compulsory to all. Morover the students should select any one of the Elective group consisting three Theory Papers and One Practical in semester III.

Old Code	New Code	Title of Course	Credits
MCE 013A	MCE 013A	Green Chemistry	4
MCE 014A	MCE 014A	Inorganic Elective I: PHOTOINORGANIC CHEMISTRY AND X-RAY DIFFRACTION	4
MCE 015B	MCE 015B	Inorganic Elective II: BIOINORGANIC CHEMISTRY	4

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MCE 016A	MCE 016A	Inorganic Elective III: ORGANOTRANSITION METAL CHEMISTRY-I	4
MCE 017A	MCE 017A	Spectrophotometric Analysis (Practical)	12
MCE 018A	MCE 018A	Organic Elective I: ORGANIC SYNTHESIS-I	4
MCE 042A	MCE 042A	Organic Elective II: HETEROCYCLIC CHEMISTRY	4
MCE 020B	MCE 020B	Organic Elective III: NATURAL PRODUCTS-I	4
MCE 021A	MCE 021A	Multi-step Synthesis (Practical)	12
MCE 022A	MCE 022A	Physical Elective I: ELECTROANALYTICAL TECHNIQUES	4
MCE 023A	MCE 023A	Physical Elective II: ELECTROCHEMISTRY-I	4
MCE 024A	MCE 024A	Physical Elective III: CHEMICAL KINETICS-I	4
MCE 025A	MCE 025A	Thermodynamical Studies (Practical)	12
			Total Credits = 28

SEMESTER – IV

A set of three elective theory papers, one Practical and a Minor Project .

Old Code	New Code	Title of Course	Credits
MCE 027A	MCE 027A	Inorganic Elective I: ORGANOTRANSITION METAL CHEMISTRY-II	4
MCE 028A	MCE 028A	Inorganic Elective II: INORGANIC POLYMERS	4
MCE 029B	MCE 029B	Inorganic Elective III: MINERAL BASED INDUSTRIAL CHEMISTRY	4
MCE 030A	MCE 030A	Flame Photometric and Flame Photometric Determination (Practical)	12
MCE 031A	MCE 031A	Organic Elective I: Disconnection Approach	4
MCE043A	MCE043A	Advanced Organic Spectroscopy	4
MCE 033C	MCE 033C	Organic Elective III: NATURAL PRODUCTS-II	4
MCE 034A	MCE 034A	Chromatography and Spectroscopy (Practical)	12
MCE 035A	MCE 035A	Physical Elective I: CHEMICAL ANALYSIS	4
MCE 036A	MCE 036A	Physical Elective II: ELECTRO CHEMISTRY-II	4
MCE 037A	MCE 037A	Physical Elective III: CHEMICAL KINETICS-II	4
MCE 038A	MCE 038A	Polarography and Chemical Kinetics (Practical)	12
MCE 041A	MCE 041A	Minor Project (Which will be done in vacations after Semester-III and will be evaluated in Semester-IV)	4
			Total Credits = 28

CREDIT SUMMARY

Sem-I	Sem-II	Sem-III	Sem-IV	Total Credits
28	28	28	28	112

Programme Outcomes

PO1.Critical Thinking: Take informed actions after identifying the assumptions that frame our thinking and actions, checking out the degree to which these assumptions are accurate and valid, and looking at our ideas and decisions (intellectual, organizational, and personal) from different perspectives.

PO2.Effective Communication: Speak, read, write and listen clearly in person and through electronic media in English and in one Indian language, and make meaning of the world by connecting people, ideas, books, media and technology.

PO3. Social Interaction: Elicit views of others, mediate disagreements and help reach conclusions in group settings.

PO4. Effective Citizenship: Demonstrate empathetic social concern and equity centred national development, and the ability to act with an informed awareness of issues and participate in civic life through volunteering.

PO5. Ethics: Recognize different value systems including your own, understand the moral dimensions of your decisions, and accept responsibility for them.

PO6. Environment and Sustainability: Understand the issues of environmental contexts and sustainable development.

PO7. Self-directed and Life-long Learning: Acquire the ability to engage in independent and life-long learning in the broadest context sociotechnological changes

Programme Specific Outcomes

PSO 1: To provide specific knowledge of chemistry at advanced level and to develop skill to understand basic concept of chemistry (Understanding skills)

PSO 2: : To educate the students to make them confident and capable of accepting any challenge in chemistry and eligibility for developing research skills. (Problem-Solving Skills)

PSO 3: To impart knowledge and understanding of the wider role of chemistry in society for creating innovative career in research and for higher studies. (Problem solving skills).

PSO 4: To understand professional responsibility and ethics in Chemistry (Intellectual skills).

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SEMESTER – I

MCE 001D: Compounds of Different Elements

After the completion of the course, student will be able to understand the:

CO-1: Basics of stereochemistry and bonding in different compounds and reactions. CO-2 The knowledge of metal- ligand bonding in complexes. CO-3 Preparation, structure, bonding, reactions and applications of Hydrogen, Alkali and Alkaline Earth Metals. CO-4 Preparation, structure and bonding of compounds of Carbon and Silicon group elements. CO-5 Types of nuclear reactions

Unit-I

Stereochemistry and Bonding in Main group compounds

VSEPR Theory, Walsh diagram. Hybridization including energetic of hybridization. Bent's rule, $d\pi-p\pi$ bond. Some simple reactions of covalently bonded molecules (i) Atomic inversion (ii) Berry pseudo rotation (iii) Nucleophilic displacement (iv) Free radical mechanism

Unit-II

Metal-Ligand bonding

Valence Bond Theory (VBT), Crystal field theory (CFT) for octahedral, trigonal bipyramidal, square pyramidal, tetrahedral and square planar complexes. Crystal field stabilization energy (CFSE), Factor affecting the crystal field parameters, weak and strong field complexes, spectrochemical series, John-Teller effect. Thermodynamic and related aspects of crystal fields - ionic radii, heats of ligation, lattice energy, site preference energy. Merits and limitations of CFT. Molecular orbital theory of octahedral, tetrahedral and square planar complexes. π bonding in bonding in octahedral complexes.

Unit-III

Hydrogen, Alkali and Alkaline Earth Metals

Classification of hydrides; e-deficient, e-precise & e-rich hydrides. Applications of crown ethers in extraction of alkali and alkaline earth metals.

Boron compounds

Preparation, structure, bonding, reactions and applications of boranes, carboranes, metalloboranes, metallocarboranes, borazines.

Noble gases

Isolation and properties. Preparation and structure of noble gas compounds

Unit-IV

Compounds of Carbon and Silicon

Fullerenes and their compounds, Intercalation compounds of graphite, Synthesis, structure, properties, and applications. Carbides, fluorocarbons, silanes, silicates, zeolites and silicones.

Compounds of Nitrogen, Oxygen and Halogen group elements **Compounds of Nitrogen, Oxygen and Halogen group elements**

Nitrogen activation. Oxidation states of nitrogen and their interconversion. BN, PN and SN

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Synthesis, properties, bonding, and applications of interhalogens, pseudohalogens, polyhalides, oxyacids and oxoanions of halogens.

Unit-V

Nuclear Chemistry: Types of radioactive decay, units of radioactivity, Nuclear reaction – evaporation, spallation, fragmentation, transfer reactions(Buckshot hypothesis) , nuclear fission: Theory of nuclear fission , fission fragments , their mass and charge distribution, fission energy, compound nucleus theory for nuclear reaction, Photonuclear reaction and nuclear fusion(thermonuclear reaction), nuclear reactors Interaction of radiation with matter. Counters – Geiger counter, scintillation counter, proportional counter, semi conductor detector. Analytical applications (neutron activation analysis and isotope dilution analysis)

Self Study: Sub-nucleons, classification of nuclides, nuclear stability, binding energy, nuclear radius, nuclear models – liquid drop model, shell model. Applications of radio isotopes as tracers: chemical investigations (structure determinations, reaction mechanism, isotope exchange reactions), age determination, medical, agricultural and industrial applications.

Suggested Books & References

1. Advanced Inorganic Chemistry, Cotton F.A. and Wilkinson G, John Wiley.
2. Inorganic Chemistry, Huhey J.E., Harper & Row.
3. Chemistry of the Elements, Greenwood N.N. and Earnshaw A., Pergamon
4. Inorganic Chemistry: A unified Approach, Porterfiels W. W., Elsevier
5. Inorganic Chemistry, Sharpe Alan G., Pearson Education Ltd.
6. Inorganic Chemistry, Shriver D.F., Atkins, P.W. and Langford C.H., Oxford University Press,1998
7. Inorganic Chemistry, Miessler G. L. and Tarr D. A., Pearson Publications
8. Inorganic Chemistry, Wulfsberg, G, University Science Books, Viva Books.

MCE 002B: Reaction Mechanism: Structure and Reactivity

Course Outcomes: On the completion of this course student will be able to-

- CO1: Understand the nature of different types of bonding associated with organic molecules.
CO2: Understand the different stereo isomers of a particular organic molecule, will be able to identify the chiral centre present in a molecule and will be able to communicate the different optical isomers with universal notation. CO3: Understand the reaction mechanism and the impact of structure on reactivity.
CO4: Understand the aliphatic nucleophilic substitution and its mechanism. CO5: Understand the photochemical reactions.

Unit-I

Nature of Bonding in Organic Molecules

Delocalized chemical bonding-conjugation, cross conjugation, resonance hyperconjugation, bonding in fullerenes, tautomerism. Aromaticity in benzenoid and non-benzenoid compounds, alternate and non-alternate hydrocarbons. Huckel's rule, energy level of p-molecular orbitals,

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Unit-II

Unit-III

Unit-IV

Unit-V

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5. Organic Chemistry, R.T. Morrison and R.N. Boyd, Prentice-Hall.
6. Modern Organic Reactions, H.O. House, Benjamin.
7. Principles of Organic Synthesis, R.O.C. Norman and J.M. Coxon, Blackie Academic & Professional.
8. Reaction Mechanism in Organic Chemistry, S.M. Mukherji and S.P. Singh, Macmillan.
9. Pericyclic Reactions, S.M. Mukherji, Macmillan, India
10. Stereochemistry of Organic Compounds, D.Nasipuri, New Age International.
11. Stereochemistry of Organic Compounds, P.S. Kalsi, New Age International.

MCE 003C: Quantum, Surface and Electro Chemistry

Course Outcome: On completion of this course student will be able to-

- CO-1 understand the postulates of quantum mechanics and derivation of Schrodinger wave equation.
- CO-2 apply and analyze the basic knowledge of various adsorption isotherms.
- CO-3 describe the basic concept of surfactants and their applications.
- CO-4 think critically on electrified double layer and different models.
- CO-5 understand practical aspects of polarography

Unit-I

Introduction to Exact Quantum Mechanical Results

The Schrodinger equation and the postulates of quantum mechanics. Operators, Hamiltonian and Hermitian operator, Discussion of solutions of the Schrodinger equation to some model systems viz., particle in a box. quantization of energy levels, degeneracy, zero point energy and justification for Heisenberg uncertainty principle, the harmonic oscillator, the rigid rotor, the hydrogen atom.

Approximate Methods

The variation theorem, linear variation principle. Perturbation theory (First order and nondegenerate). Applications of variation method and perturbation theory to the Helium atom.

Unit-II

Molecular Orbital Theory, LCAO Concept. Extension of MO theory to homonuclear and heteronuclear diatomic molecules, Qualitative MO theory and its applications to AH_2 type molecule, Huckel theory of conjugate systems, bond order and charge density calculations. Applications to ethylene, butadiene, cyclobutadiene, benzene, allyl system and cyclopropenyl system. Introduction to extended Huckel theory.

Unit-III

Surface Chemistry

Surface tension, capillary action, pressure difference across curved surface (Laplace equation), vapour pressure of droplets (Kelvin equation), Gibbs adsorption isotherm, estimation of surface area (BET equation), Surface films on liquids (Electro-kinetic phenomenon).

Micelles

Surface active agents, classification of surface active agents, micellization, hydrophobic interaction, critical micellar concentration (CMC), factors affecting the CMC of surfactants,

21-


counter ion binding to micelles, thermodynamics of micellization-phase separation and mass action models, solubilization, micro emulsion, reverse micelles.

Unit-IV

Electrochemistry

Electrochemistry of solutions. Debye-Huckel-Onsager treatment and its extension, ion solvent interactions. Thermodynamics of electrified interface equations. Derivation of electrocapillarity, Lippmann equations (surface excess), methods of determination. Structure of electrified interfaces. Gouy-Chapman, Stern, Grahm-Devanathan-Mottwatts, Tobin, Bockris, Devanathan model.

Unit-V

Overpotential

Introduction, types of overpotential, theories, exchange current density, introduction of Butler Volmer equation, Tafel plot. Semiconductor interfaces-theory of double layer at semiconductor, electrolyte solution interfaces, Effect of light at semiconductor solution interface. Polarography theory, Ilkovic equation; half wave potential and its significance.

Suggested Books & References:

1. Physical Chemistry, P.W. Atkins, ELBS.
2. Introduction to Quantum Chemistry, A.K. Chandra, Tata Mc Graw Hill.
3. Quantum Chemistry, Ira N. Levine, Prentice Hall.
4. Coulson's Valence, R. Mc Weeny, ELBS.
5. Chemical Kinetics, K.J. Laidler, McGraw-Hill.
6. Kinetics and Mechanism of Chemical Transformation J. Rajaraman and J. Kuriacose, Mc Millan.
7. Micelles, Theoretical and Applied Aspects, V. M. Rao, Plenum.
8. Modern Electrochemistry Vol. I and Vol II J.O.M. Bockris and A.K.N. Reddy, Plenum.
9. Introduction to Polymer Science, V.R. Gowarikar, N.V. Vishwanathan and J. Sridhar, Wiley Eastern.

MCE 004B: Mathematics and Computers for Chemists

Course Objectives: This course has the following objectives:

CO1 To teach students the addition and multiplication; inverse, adjoint and transpose of matrices, special matrices and their properties. Homogeneous, non-homogeneous linear equations and conditions for the solution, linear dependence and independence. eigenvalues and eigenvectors, diagonalization, determinants.

CO2 To expose students to the Functions, continuity and differentiability, rules for differentiation, applications of differential calculus including maxima and minima, Integral calculus, basic rules for integration.

CO3 To expose students basics of First-order and first degree differential equations and their applications. Second order differential equation and their solutions.

CO4 To teach students 'Introduction to computers, Basic structure and functioning of computer with a PC as illustrative example. Memory I/O devices. Secondary storage Computer languages. Operating systems.

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COSTo teach students Computer Programming in C, History of "C", operators and expression, input & output operation, decision making and branching looping, arrays, function, structures and unions.

Unit-I

Matrix Algebra.

Addition and multiplication; inverse, adjoint and transpose of matrices, special matrices (Symmetric, skew-symmetric, Hermitian, Skey-Harmitian, unit, diagonal, unitary etc.) and their properties. Matrix equations: Homogeneous, non-homogeneous linear equations and conditions for the solution, linear dependence and independence. Introduction to vector spaces, matrix eigenvalues and digenvetors, diagonalization, determinatnts (examples from Juckel theory).

Unit-II

Differential Calculus

Functions, continuity and differentiability, rules for differentiation, applications of differential calculus including maxima and minima (examples related to maximally populated rotational energy levels, Bohr's radius and most probable velocity from Maxwell's distribution etc.). Integral calculus, basic rules for integration, integration by parts, partial fractions and substitution. Reduction formulae, applications of integral calculus. Functions of several variables, partial differentiation, co-ordinate transformations (e.g. cartesian to spherical polar).

Unit-III

Elementary Differential equations

First-order and first degree differential equations, homogenous, exact and linear equations. Applications to chemical kinetics, secular equilibria, quantum chemistry etc. second order differential equation and their solutions.

Unit-IV

Introduction to computers

Basic structure and functioning of computer with a PC as illustrative example. Memory I/O devices. Secondary storage Computer languages. Operating systems Introduction to UNIX and WINDOWS. Principles of programming Alogrithms and flow-charts.

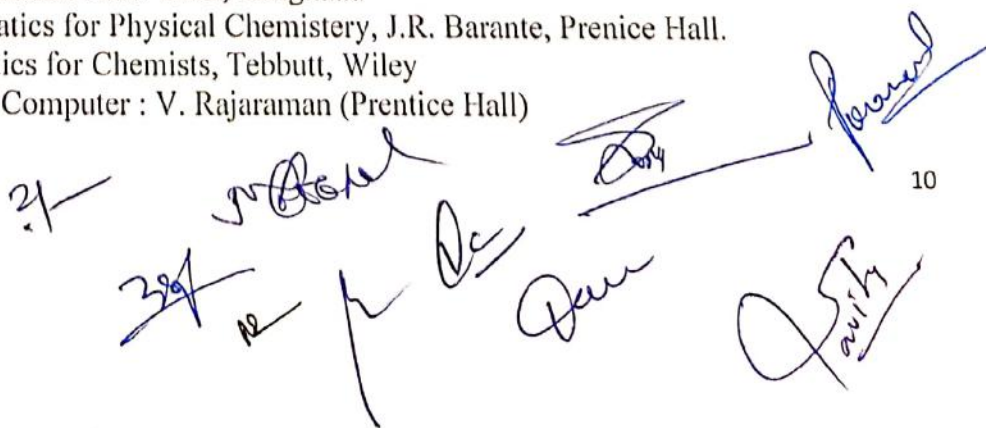
Unit-V

Computer Programming in C

History of "C" constants, variables and data types, operators and expression, input & output operation, decision making and branching looping, arrays, function, structures and unions, Program with data preferably from physical chemistry Laboratory. Introduction of working of LOTUS/EXCEL/FOXPRO/MOPAC and word processing softwares.

Suggested Books & References:

1. The chemistry Mathematics Book, E.Steiner, Oxford University Press.
2. Mathematifs for chemistry, Doggett and Suiclific, Logman.
3. Mathematical for Physical chemistry : F. Daniels, Mc. Graw Hill.
4. Chemical Mathematics D.M. Hirst, Longman.
5. Applied Mathematics for Physical Chemistery, J.R. Barante, Prenice Hall.
6. Basic Matchematics for Chemists, Tebbutt, Wiley
7. Fundamentals of Computer : V. Rajaraman (Prentice Hall)



8. Computers in Chemistry E. V. Ramana (Tata Mc Graw Hill)
9. Computer Programming in FORTRAN IV. V. Rajaraman (Prentice Hall)

MCE 005A: Qualitative and Quantitative Analysis (Practical)

Inorganic Chemistry

1. To identify acidic radicals of dilute H_2SO_4 group.
2. To identify acidic radicals of concentrated H_2SO_4 group.
3. To identify acidic radicals not identify with dilute or concentrated H_2SO_4 group.
4. To analyze basic radicals of group I and II.
5. To analyze basic radicals of group III and IV.
6. To analyze basic radicals of group V, VI and VII.
7. To analyze less common metal ions Ti, Mn, W, Fe, Zr, Th, V, U.
8. Analysis of the mixture number 1 containing four acidic and four basic radicals.
9. Analysis of the mixture number 2 containing four acidic and four basic radicals.
10. Analysis of the mixture number 3 containing four acidic and four basic radicals.
11. Analysis of the mixture number 4 containing four acidic and four basic radicals.
12. Qualitative Analysis: Separation and determination of two metal ions Cu-Ni involving volumetric and gravimetric methods.
13. Qualitative Analysis: Separation and determination of two metal ions Ni-Zn involving volumetric and gravimetric methods.
14. Qualitative Analysis: Separation and determination of two metal ions Cu-Fe etc. involving volumetric and gravimetric methods.

Organic Chemistry

1. To separate and identify the organic mixture containing two solid components using water and prepare their suitable derivatives.
2. To separate and identify the organic mixture containing two solid components using hot water and prepare their suitable derivatives.
3. To separate and identify the organic mixture containing two solid components using NaOH and prepare their suitable derivatives.
4. To separate and identify the organic mixture containing two solid components using $NaHCO_3$ and prepare their suitable derivatives.
5. To separate and identify the organic mixture number 1 containing one solid and one liquid components and prepare their suitable derivatives.
6. To separate the mixture of Methyl Orange and Methylene Blue by using cyclohexane and ethyl acetate (8.5:1.5) as solvent system.
7. Preparation and separation of 2,4-dinitro Phenylhydrazone of acetone, 2-butanone using toluene and petroleum ether (40:60).
8. Preparation and separation of 2,4-dinitro Phenylhydrazone of hexane-2-one and hexane-3-one using toluene and petroleum ether (40:60).

29-


9. To separate the mixture of phenylalanine and glycine. Alanine and aspartic acid. Leucine and glutamic acid. Spray reagent - Ninhydrin.
10. To separate the mixture of D,L-alanine, glycine and L-leucine using n-butanol : acetic acid : water (4:1:5) Spray reagent - Ninhydrin.
11. To separate monosaccharides - a mixture of D-galactose and D-fructose using n-butanol : acetone : water (4:1:5) Spray reagent - aniline hydrogen phthalate.
12. Determination of DO, COD and BOD of water sample.

Physical Chemistry

1. Calibration of volumetric apparatus, burette, pipette and standard flask.
2. To investigate the adsorption of oxalic acid from aqueous solution by activated charcoal, and examine the validity of Freundlich and Langmuir adsorption isotherm.
3. To investigate the adsorption of acetic acid from aqueous solution by activated charcoal, and examine the validity of Freundlich and Langmuir adsorption isotherm.
4. Determination of congruent composition and temperature of a binary system (e.g. diphenylamine-benzophenone system).
5. Determination of glass transition temperature of given salt (e.g., CaCl_2) conductometrically.
6. To construct the phase diagram for three component system (e.g. chloroform-acetic acid-water).
7. To construct the phase diagram for three component system (e.g. alcohol-benzene-water).
8. To determine CST of phenol and water in presence of 1.0% NaCl, 0.5% naphthalene, 1% succinic acid.
9. Determination of the velocity constant, order of the reaction and energy of activation for saponification of ethyl acetate by sodium hydroxide conductometrically.
10. Determination of solubility and solubility product of sparingly soluble salts e.g. PbSO_4 , BaSO_4) conductometrically.
11. Determination of the strength of strong and weak acid in a given mixture conductometrically.
12. To study of the effect of solvent on the conductance of AgNO_3 /acetic acid and to determine the degree of dissociation and equilibrium constant in different solvents and in their mixtures (DMSO, DMF, dioxane, acetone, water) and to test the validity of Debye-Huckel-Onsager theory.
13. Determination of the activity coefficient of zinc ions in the solution of 0.002 M zinc sulphate using Debye Huckel's limiting law.

Books Suggested

1. Vogel's Textbook of Quantitative Analysis, revised, J. Bassett, R.C. Denney, G.H. Jeffery and J. Mendham, ELBS.
2. Synthesis and Characterization of Inorganic Compounds, W.L. Jolly. Prentice Hall.
3. Experiments and Techniques in Organic Chemistry, D.P. Pasto, C. Johnson and M. Miller, Prentice Hall.
4. Macroscale and Microscale Organic Experiments, K.L. Williamson, D.C. Heath.
5. Systematic Qualitative Organic Analysis, H. Middleton, Edward Arnold.
6. Handbook of Organic Analysis-qualitative and Quantitative. H. Clark, Edward Arnold.

21-
297
J. Bassett
R. C. Denney
G. H. Jeffery
J. Mendham
W. L. Jolly
D. P. Pasto
C. Johnson
M. Miller
K. L. Williamson
D. C. Heath
H. Middleton
H. Clark

12

7. Vogel's Textbook of Practical Organic Chemistry, A.R. Tatchell, John Wiley.
8. Practical Physical Chemistry, A.M. James and F.E. Prichard, Longman.
9. Findley's Practical Physical chemistry, B.P. Levitt, Longman.
10. Experimental Physical Chemistry, R.C. Das and B. Behera, Tata McGraw Hill.

SEMESTER II

MCE 007B: Chemistry of Transition Metals

Course Outcome: After the completion of the course, student will be able to understand:

CO1: metal-ligand bonding through different theories and metal-ligand equilibria in solution and their relative stability.

CO2 electronic spectra and calculation of different parameters.

CO3 energy profile and reaction mechanism of transition metal complexes and different types of reactions like substitution, redox *etc.* and related theories.

CO4 Symmetry, symmetry elements, orthogonality theorem and group theory of molecules.

CO5 to apply the knowledge of group theory on different molecules and systems..

Unit-I

Metal ligand Equilibria in solution

Stepwise and overall formation constants and their interaction, trends in stepwise constants. Factors affecting stability of metal complexes with reference to the nature of metal ion and ligand chelate effect and its thermodynamic origin. Determination of binary formation constant by pHmetry and spectrophotometry.

Unit-II

Electronic spectra of transition metal complexes

Types of electronic transition, selection rules for d-d transitions. Spectroscopic ground states, correlation. Orgel and Tanabe-Sugano diagrams for transition metal complexes. Calculation of Racah parameters. Charge transfer spectra.

Unit-III

Reaction mechanism of transition metal complexes

Energy profile of a reaction, reactivity of metal complex, inert and labile complexes, kinetics of octahedral substitution, acid hydrolysis, factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism, direct and indirect evidences in favour of conjugate mechanism, anation reactions, reactions without metal ligand bond cleavage.

Substitution reactions in square planar complexes, the trans effect, mechanism of the substitution reaction. Redox reaction, electron transfer reactions, mechanism of one electron transfer reactions, outer sphere type reactions, cross reactions and Marcus-Hush theory, inner sphere type reactions.

13

Unit-IV

Symmetry and Group Theory

Symmetry elements and symmetry operations, definition of group and subgroup, conjugacy relation and classes, product of symmetry operations, relation between symmetry elements and symmetry operations, orders of a finite group and its subgroup, point group symmetry, schonflies symbols, representations of groups by reducible and irreducible presentations and relation between them (representation for the C_n , C_{nv} , D_{nh} etc. groups to be worked out explicitly), character of a representation, the great orthogonality theorem (without proof) and its importance, character tables of C_{2v} and C_{3v} and their use.

UNIT V

Applications of Group Theory in Chemistry

Formation of hybrid orbitals: sigma bonding in linear structure ($BeCl_2$), trigonal planar (BF_3), tetrahedral (CH_4), square pyramid (BrF_5) and square planar (XeF_4), octahedral and square planar complexes, π bonding in complex compounds: square planar molecule and tetrahedral molecule. Molecules with delocalized- π orbitals, cyclopropenyl system, cyclobutenyl system, cyclopentadienyl system and benzene.

Suggested Books & References:

1. Advanced Inorganic Chemistry, Cotton F.A., Wilkinson G., Murillo C.A. Bochmann M., John Wiley
2. Inorganic Chemistry, Huheey J.E., Harper & Row.
3. Chemistry of the Elements. Greenwood N.N. and Earnshaw A., Pergamon.
4. Inorganic Electronic Spectroscopy, Lever A.B.P., Elsevier.
5. Magnetochemistry, Carlin R.I., Springer Verlag.
6. Inorganic Chemistry, Willyberg G, University Science Books.
7. Chemical Bonding by Patel & Patel, Vallabh Vidyanagar
8. Chemical Applications of Group Theory by F. Albert Cotton, Wiley.
9. Symmetry and Structure: Readable Group Theory for Chemists By Sidney F. A. Kettle, Wiley
10. Molecular symmetry and group theory by Robert L. Carter, Wiley
11. Introduction to the Chemical Applications of Group Theory by L E Laverman
12. Group Theory Applied to Chemistry (Theoretical Chemistry and Computational by Arnout Jozef Ceulemans
13. Group Theory and its Chemical Applications by Bhattacharya P.K., Himalaya Publishing House

MCE 008A: Reaction mechanism: Addition, Elimination and Pericyclic Reactions

Course Outcome: After the completion of the course, student will be able to understand:

CO-1: different aromatic nucleophilic substitution and free radical reactions. CO-2 aliphatic and aromatic electrophilic substitution reactions. CO-3 mechanistic and stereochemical aspects of addition to C-C

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14

multiple bonds. CO-4 mechanism of C-bonders multiple bonds and elimination reactions CO-5 symmetry, types and rearrangement of pericyclic reactions.

Unit - I

Aromatic Nucleophile Substitution

The S_NA_r SN1, benzyne and SN1 mechanism, Reactivity effect of substrate structure, leaving group and attacking nucleophile. The Von Richter, Sommelet-Hauser, and Smiles rearrangements.

Free Radical Reactions

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

Unit - II

Aliphatic Electrophilic Substitution

Bimolecular mechanisms SE2 and SE1, The SE1 mechanism, electrophilic substitution accompanied by double bond shifts. Effect of substrates, leaving groups and the solvent polarity on the reactivity.

Aromatic Electrophilic Substitution

The arenium ion mechanism, orientation and reactivity, energy profile diagrams. The ortho/para ratio, ipso attack, orientation in other ring systems. Quantitative treatment of reactivity in substrates and electrophiles. Diazonium coupling, Vilsmeier reaction, Gatterman-Koch reaction.

Unit - III

Addition to Carbon-Carbon Multiple Bonds :

Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, regio- and chemoselectivity, orientation and reactivity. Addition to cyclopropane ring. Hydrogenation of double and triple bonds, hydrogenation of aromatic rings. Hydroboration, Michael reaction, Sharpless asymmetric epoxidation.

Unit-IV

Addition to Carbon-Hetero Multiple bonds

Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acid esters and nitriles. Addition of Grignard reagents, Organozinc and Organolithium reagents to carbonyl and unsaturated carbonyl compounds. Wittig reaction. Mechanism of condensation reactions involving enolates-Aldol, Knoevenagel, Claisen, Mannich, Benzoin, Perkin and Stobbe reactions. Hydrolysis of esters and amides, ammonolysis of esters.

Elimination Reactions

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

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Pericyclic Reactions

Suggested Books & References:

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

Course outcomes: After the completion of the course, student will be able to understand the:

CO-2 criteria for statistical and non equilibrium thermodynamics.

CO-3 translation, rotational, vibrational and electronic partition functions and molar quantities.

CO-4 rate laws, collision theory of reaction rates, Arrhenius equation and the activated complex theory.

CO-5 kinetics of enzyme catalyzed reactions, fast and unimolecular reactions.

Classical Thermodynamics

Classical Thermodynamics
Concepts of laws of thermodynamics, free energy, chemical potential and entropies. Partial molar free energy, partial molar volume and partial molar heat content and their significance. Determinations of these quantities. Concept of fugacity and determination of fugacity, activity, activity coefficient, determination of activity and activity coefficients.

Unit II

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Concept of distribution, thermodynamic probability and most probable distribution. Ensemble averaging, postulates of ensemble averaging. Canonical, grand canonical and microcanonical ensembles, corresponding distribution laws (using Lagrange's method of undetermined multipliers). Thermodynamic criteria for non equilibrium states, entropy production and entropy flow, transformation of generalized forces and forces, non equilibrium stationary states, phenomenological equations, Onsager's reciprocity relations.

Unit III

Partition Functions

Partition functions-translation, rotational, vibrational and electronic partition functions, Fermi-Dirac Statistics, Maxwell distribution law and applications to metal, Bose-Einstein statistics distribution Law and application to helium, Partition molar quantities in term of thermodynamic functions.

Unit IV

Chemical Dynamics-I

Methods of determining rate laws, collision theory of reaction rates, steric factor, activated complex theory, Arrhenius equation and the activated complex theory; ionic reactions, kinetic salt effects, steady state kinetics, kinetic and thermodynamic control of reactions, Dynamic chain reaction (hydrogen-bromine reaction, pyrolysis of acetaldehyde, decomposition of ethane), photochemical reaction (hydrogen-bromine and hydrogen-chlorine reactions), Oscillatory reactions: Belousov-Zhabotinsky reaction.

Unit V

Chemical Dynamics-II

Kinetics of enzyme catalyzed reactions, general features for fast reactions, study of fast reactions by flow method, relaxation method, flash photolysis and the nuclear magnetic resonance method, dynamics of unimolecular reactions (Lindemann Hinshelwood, Rice-Ramsperger and Kassel theories and Marcus (RRKM) theories for unimolecular reactions).

Suggested Books & References:

1. Physical Chemistry, P.W. Atkins, ELBS.
2. Introduction to Quantum Chemistry, A.K. Chandra, Tata Mc Graw Hill.
3. Quantum Chemistry, Ira N. Levine, Prentice Hall.
4. Coulson's Valence, R. Mc Ween y, ELBS.
5. Chemical Kinetics. K.J. Laidler, McGraw-Hill.
6. Kinetics and Mechanism of Chemical Transformation J. Rajaraman and J. Kuriacose, Mc Millan.
7. Micelles, Theoretical and Applied Aspects, V. M. Rao, Plenum.
8. Modern Electrochemistry Vol. I and Vol II J.O.M. Bockris and A.K.N. Reddy, Plenum.
9. Introduction to Polymer Science, V.R. Gowarikar, N.V. Vishwanathan and J. Sridhar, Wiley Eastern.

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MCE 010C: Applications of Spectroscopy

Course Outcomes: After the completion of the course, student will be able to-
CO1 Understand the common terms and principles in spectroscopy. Principles of UV spectroscopy, its applications in structure determination and working method of Instrument.
CO2 Understand the Principles IR spectroscopy and Raman spectroscopy, their applications in structure determination and working method of Instrument.
CO3 Understand the principles of Rotational spectroscopy, ESR spectroscopy, their applications in structure determination and working method of Instrument.
CO4 Understand the basic principle Principles of NMR Spectroscopy, instrumentation and applications. Student will also learn about the use of NMR technique in medical sciences.
CO5 Understand the basic principles of Photoelectron spectroscopy, Electron microscopy and their applications in structure determination and working method of Instrument. Student will also learn about chromatographic techniques.

Unit-I

Basic Elements of Spectroscopy

Uncertainty relation and natural line width, natural line broadening, doppler line broadening, pressure broadening, saturation broadening, removal of line broadening, signal-to-noise ratio, resolving power, intensity of spectral lines – transition probability, population of states, path length of sample. General components of an absorption experiment in various regions, dispersing elements, basic elements of practical spectroscopy, Born-Oppenheimer approximation: derivations, Fourier Transform methods (IR and NMR)

Ultraviolet and Visible spectroscopy

Various electronic transitions (185-800 nm) Beer-Lambert law, effect of solvent on electronic transitions, ultraviolet bands for carbonyl compounds, unsaturated carbonyl compounds, dienes, conjugated polyenes, Fiesher -Woodward rules for conjugated dienes and carbonyl compounds, ultraviolet spectra of aromatic compounds. Steric effect in biphenyls.

Unit-II

Infrared Spectroscopy

Instrumentation and Sample handling. Characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ether's, phenols and amines, and carbonyl compounds (ketones, aldehydes, esters, amides, acids, anhydrides, lactones, lactams and conjugated carbonyl compounds). Effect of hydrogen bonding and solvent effect on vibrational frequencies, overtones, combination bands and fermi resonance.

Raman Spectroscopy

Principle, stokes-antistokes lines, raman effect, applications, Coherent Antistokes Raman Spectroscopy CARS (an elementary idea), Raman spectroscopy particularly for the study of active sites of metalloproteins

Unit-III

Rotational Spectroscopy. Classification of molecules, linear triatomic molecule, intensities, energy levels and rotational spectra of symmetric top molecules, Stark effect, nuclear and electron spin interaction, effect of external field, applications.

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Electron Spin Resonance Spectroscopy

Some basic elements of ESR spectroscopy, relaxation processes: spin-lattice relaxation, spin-spin relaxation and exchange interaction. Zero field splitting and Kramer's degeneracy, 'g' value and factors affecting ESR lines.

Unit-IV

Nuclear Magnetic Resonance Spectroscopy General introduction and definition, chemical shift, spin-spin interaction, shielding mechanism of measurement, chemical shift values and correlation for protons bonded to carbon and other nuclei, chemical exchange, effect of deuteration, complex spin-spin interaction between two, three, four and five nuclei (first order spectra). NMR shift reagents, solvent effects, Nuclear Overhauser effect (NOE), Introduction of Mass Spectrometry, NQR Spectroscopy, Introduction of Mössbauer spectroscopy.

Unit-V

Photoelectron Spectroscopy

Basic principle, ionization process, Koopmen's theorem, photoelectron spectra of simple molecules, ESCA and its applications, Auger electron spectroscopy (basic idea), spectra of transition metal complexes, charge transfer spectra.

Electron Microscopy

Basic principles of Electron Microscopy: SEM, TEM and their applications in structural analysis

Suggested Books & References:

1. Physical Methods for Chemistry, R.S. Drago, Saunders Compnay.
2. Structural Methods in Inorganic Chemistry, E.A.V. Ebsworth, D.W.H. Rankin and S. Cradock, ELBS.
3. Infrared and Raman Spectral : Inorganic and Coordination Compounds K. Nakamoto, Wiley.
4. Progress in Inorganic Chemistry vol., 8, ed., F.A. Cotton, vol., 15 ed. S.J. Lippard, Wiley.
5. Transition Metal Chemistry ed. R.L. Carlin vol. 3 dekker.
6. Inorganic Electronic Spectroscopy, A.P.B. Lever, Elsevier.
7. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, .V. Parish, Ellis Haywood.
8. Practical NMR Spectroscopy, M.L. Martin. J.J. Deepish and G.J. Martin, Heyden.
9. Spectrometric Identification of Organic Compounds, R.M. Silverstein, G.C. Bassler adn T.C. Morrill, John Wiley.
10. Introduction to NMR spectroscopy, R.J. Abraham, J. Fisher and P. Loftus, Wiley.
11. Application of Spectroscopy of Organic Compounds, J.R. Dyer Prentice Hall.
12. Spectroscopic Methods in Organic Chemistry D.H. Williams, I. Fleming, Tata McGraw-Hill.

MCE 011A: Chromatographic Separations, Organic Synthesis and Potentiometric Analysis (Practical)

INORGANIC CHEMISTRY

A. Chromatography Separation of cations and anions by

1. Paper Chromatography.
2. Chromatography : Ion exchange.

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B. Chromatographic Separations

3. Cadmium and zinc
4. Zinc and magnesium.
5. Thin-layer chromatography-separation of nickel, manganese, cobalt and zinc. Determination of R_f values.
6. Separation and identification of the sugars present in the given mixture of glucose, fructose and sucrose by paper chromatography and determination of R_f values.

C. Preparations(Any Six)

Preparation of selected inorganic compounds and their studies by I.R. electronic spectra, Mossbauer, E.S.R. and magnetic susceptibility measurements. Handling of air and moisture sensitive compounds.

1. $\text{VO}(\text{acac})_2$
2. $\text{TiO}(\text{C}_9\text{H}_8\text{NO})_2 \cdot 2\text{H}_2\text{O}$
3. $\text{cis-K}[\text{Cr}(\text{C}_2\text{O}_4)_2(\text{H}_2\text{O})_2]$
4. $\text{Na}[\text{Cr}(\text{NH}_3)_2(\text{SCN})_4]$
5. $\text{Ni}(\text{acac})_2$
6. $\text{K}_3[\text{Fe}(\text{C}_2\text{O}_4)_3]$
7. Prussian Blue, Turnbull's Blue.
8. $[\text{Co}(\text{NH}_3)_6][\text{Co}(\text{NO}_2)_6]$
9. $\text{cis-}[\text{Co}(\text{trien})(\text{NO}_2)_2]\text{Cl} \cdot \text{H}_2\text{O}$
10. $\text{Hg}[\text{Co}(\text{SCN})_4]$
11. $[\text{Co}(\text{Pv})_2\text{Cl}_2]$
12. $[\text{Ni}(\text{NH}_3)_6]\text{Cl}_2$
13. $\text{Ni}(\text{dmg})_2$
14. $[\text{Cu}(\text{NH}_3)_4]\text{SO}_4 \cdot \text{H}_2\text{O}$

ORGANIC CHEMISTRY

Organic Synthesis

1. Acetylation : Acetylation of cholesterol and separation of cholesteryl acetate by column chromatography.
2. Oxidation : Adipic acid by chromic acid oxidation of cyclohexanol
3. Grignard reaction : Synthesis of triphenylmethanol from benzoic acid
4. Aldol condensation : Dibenzal acetone from benzaldehyde.
5. Sandmeyer reaction : p-Chlorotoluene from p-toluidine.
6. Acetoacetic ester Condensation : Synthesis of ethyl-n-butylacetoacetate by A.E.E. condensation.
7. Cannizzaro reaction : 4-Chlorobenzaldehyde as substrate.
8. Friedel Crafts reaction : benzoyl propionic acid from succinic anhydride and benzene.
9. Aromatic electrophilic substitutions : Synthesis of p-nitroaniline and p-bromoaniline.
10. Estimation of amines/phenols using bromate bromide solution/or acetylation method.
11. Determination of the percentage or number of hydroxyl groups in an organic compound by acetylation method
12. Determination of Iodine and Saponification values of an oil sample.

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PHYSICAL CHEMISTRY

1. Determination of the effect of (a) Change of temperature (b) Change of concentration of reactant and catalyst and (c) Ionic strength of the media on the velocity constant of hydrolysis of an ester/ionic reaction.
2. Determination of the velocity constant of hydrolysis of an ester/ionic reaction in micellar media.
3. Determination of the velocity constant for the oxidation of iodide ions by hydrogen peroxide study the kinetics as an iodine clock reactions.
4. Flowing clock reactions (Ref : Experiments in Physical Chemistry by Showmaker)
5. Determination of the primary salt effect on the kinetics of ionic reaction and testing of the Bronsted relationship (iodide ion is oxidised by persulphate ion).
6. To determine the relative strength of the acids by studying the hydrolysis of an ester. (at room and at any higher temperature)
7. Determine the energy of activation for the hydrolysis of an ester.
8. Determination of molecular weight of non-volatile and electrolyte/electrolyte by cryoscopic method and to determine the activity coefficient of an electrolyte.
9. Determination of the degree of dissociation of weak electrolyte and to study the deviation from ideal behaviour that occurs with a strong electrolyte.
10. Determination of strengths of halides in a mixture potentiometrically.
11. Determination of the strength of strong and weak acids in a given mixture using a potentiometer/pH meter.
12. Determination of temperature dependence of EMF of a cell.
13. Determination of the formation constant of silver-ammonia complex and stoichiometry of the complex potentiometrically.
14. Determination of rate constant for hydrolysis/inversion of sugar using a polarimeter.

Books Suggested

1. Vogel's Textbook of Quantitative Analysis, revised, J. Bassett, R.C. Denney, G.H. Jeffery and J. Mendham, ELBS.
2. Synthesis and Characterization of Inorganic Compounds, W.L. Jolly. Prentice Hall.
3. Experiments and Techniques in Organic Chemistry, D.P. Pasto, C. Johnson and M. Miller, Prentice Hall.
4. Macroscale and Microscale Organic Experiments, K.L. Williamson, D.C. Heath.
5. Systematic Qualitative Organic Analysis, H. Middleton, Edward Arnold.
6. Handbook of Organic Analysis-qualitative and Quantitative. H. Clark, Edward Arnold.
7. Vogel's Textbook of Practical Organic Chemistry, A.R. Tatchell, John Wiley.
8. Practical Physical Chemistry, A.M. James and F.E. Prichard, Longman.
9. Findley's Practical Physical chemistry, B.P. Levitt, Longman.
10. Experimental Physical Chemistry, R.C. Das and B. Behera, Tata McGraw Hill.

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Semester III

MCE 013A: Green Chemistry

Course Outcomes: After the completion of the course, student will be able to-

- CO1 Understand the twelve principles of green chemistry with their explanations and examples.
- CO2 Understand the Prevention of waste/byproducts, Prevention/Minimization of hazardous/toxic products, & designing safer chemicals - different basic approaches, Designing biodegradable products.
- CO3 Understand the Introduction of microwave induced organic and inorganic synthesis; microwave activation equipment; time and energy benefits; limitations;
- CO4 Understand the use of ionic liquids as green solvents, Electrochemical synthesis.
- CO5 Understand Oxidation-reduction reagents and catalysts; multifunctional reagents; Combinatorial green chemistry, solventless reactions, Noncovalent derivatization, Biomass conversion, emission control, Biocatalysis.

Unit-I

INTRODUCTION, PRINCIPLE AND CONCEPTS OF GREEN CHEMISTRY:

What is green chemistry? Need for green chemistry; inception and evolution of green chemistry; twelve principles of green chemistry with their explanations and examples; designing a green synthesis using these principles; green chemistry in day to day life.

Unit-II

Basic principles of Green Chemistry and their illustrations with examples.

- (i) Prevention of waste/byproducts.
- (ii) Maximum Incorporation of the materials used in the process into the final product (Atom Economy): Green metrics
- (iii) Prevention/Minimization of hazardous/toxic products.
- (iv) Designing safer chemicals - different basic approaches
- (v) Selection of appropriate auxiliary substances (solvents, separation agents etc)
- (vi) Energy requirements for reactions—use of microwave, ultrasonic energy
- (vii) Selection of starting materials—use of renewable starting materials.
- (viii) Avoidance of unnecessary derivatization—careful use of blocking/protection groups.
- (ix) Use of catalytic reagents (wherever possible) in preference to stoichiometric reagents.
- (x) Designing biodegradable products.
- (xi) Prevention of chemical accidents.
- (xii) Strengthening/development of analytical techniques to prevent and minimize the generation of hazardous substances in chemical processes. Development of accurate and reliable sensors and monitors for real time in process monitoring.

Unit-III

Application of non conventional energy sources :Microwave induced and ultrasound assisted green synthesis.

Introduction of microwave induced organic and inorganic synthesis; microwave activation – equipment; time and energy benefits; limitations;

- (a) Synthesis of nitrogen-oxygen /sulphur donor ligands and their coordination complexes
- ;synthetic organic transformations under microwaves.

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(b) Reactions in organic solvents –esterifications ,Fries rearrangement,Diels alder reaction and decarboxylation.

(c) Solvent free reactions(solid state reactions):deacetylation ;deprotection; saponification of ester;alkylation of reactive methylene compounds ;synthesis of nitriles from aldehydes; heterocyclic synthesis –B-lactams,pyrrole,quinoline. Ultrasound assisted green synthesis:introduction;instrumentation;physical aspects;oxidation;reduction;addition ,substitution reactions and synthesis of chromenes.

Unit-IV

Environmentally benign solutions to organic solvents(focus on water and ionic liquids).

(a) Ionic liquids as green solvents –Introduction ;properties and types of ionic liquids; synthetic applications-Diels-Alder reaction ;epoxidation;Heck reaction;preparation of pharmaceutical compounds;enzyme catalysed synthesis.

(b) Aqueous phase reactions-introduction;Pseudo organic solvent

(1) Application in oxidation of nitro;aromatic and carbonyl compounds;reduction of carbon-carbon multiple bond,Benzoin condensation;Michael reaction;Claisen rearrangement;knoevenagel reaction.

(2) Electrochemical synthesis- introduction,synthesis of sebacic acid,adiponitrile introduction on role of fluoros solvents and supercritical carbon dioxide in green chemistry .

Unit-V

Hazard assessment and mitigation in chemical industry

Future trends in Green Chemistry: Oxidation-reduction reagents and catalysts; Biomimetic, multifunctional reagents; Combinatorial green chemistry; Proliferation of solventless reactions; Noncovalent derivatization. Biomass conversion, emission control. Biocatalysis

Suggested Books References:

1. Organic synthesis in water, Paul A. Grieco Blackie.
2. Green Chemistry, theory and practice, Paul T. Anastas and John C. Warner.
3. New Trends in Green Chemistry,V.K. Ahluwalia and M.Kidwai.
4. Green Chemistry For Sustainability, Sanjay K. Sharma and A.Mudhoo, CRC Taylor & Francis,. USA
5. Organic synthesis: Special techniques, V.K. Ahluwalia and Renu Aggarwal.
6. A Handbook of Applied Biopolymer Technology, Sanjay K. Sharma and A. Mudhoo, RSC Publishing, UK
7. Lancaster, M. Green chemistry; An Introductory Text; the Royal Society of Chemistry: Cambridge, UK, 2002.
8. Green Corrosion Chemistry & Engineering, Sanjay K. Sharma, Wiley Publications, UK
9. Chem, Rev. 2007, 107, 2167-2820 (special issue on green chemistry).

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Specialization: Inorganic Chemistry

MCE 014A: Inorganic Elective I: PHOTONORGANIC CHEMISTRY AND X-RAY DIFFRACTION

Course outcome: After the completion of the course, student will be able to-

CO1 understand basics of photochemistry including various excitations and energy dissipation.

CO2 articulate the photochemical kinetics for radiative processes and deactivation of molecules by quenching.

CO3 understand the different photochemical reactions viz. reduction, oxidation, substitution at ground and excited level.

CO4 understand the mechanisms of electron relay, water photolysis, nitrogen fixation and CO₂ reduction.

CO5 understand the applications of XRD, methods of structural analysis of crystal, diffraction pattern etc.

Unit-I

Basic of Photochemistry

Absorption, excitation, photochemical laws, quantum yield, electronically excited states-life times-measurements of the times. Flash photolysis, Energy dissipation by radiative and non-radiative processes, absorption spectra, Frank-Condon principle, photochemical stages-primary and secondary processes.

Unit-II

Properties of Excited States

Structure, dipole moment, acid-base strengths, reactivity. Photochemical kinetics-calculation of rates of radiative processes. Bimolecular deactivation-quenching.

Excited States of Metal Complexes

Excited states of metal complexes : Comparison with organic compounds, electronically excited states of metal complexes, charge transfer spectra.

Unit-III

Ligand Field Photochemistry

Photosubstitution, photooxidation and photoreduction, lability and selectivity, zero vibrational levels of ground state and excited state.

Unit-IV

Metal Complex Sensitizers

Metal complex sensitizer, electron relay, metal colloid systems, water photolysis, nitrogen fixation and carbon dioxide reduction.

Unit-V

X-RAY DIFFRACTION

Bragg condition, Miller indices, Laue Method, Bragg method, Debye Scherrer method of X-ray structural analysis of crystals, index reflections, identification of unit cells from systematic absences in diffraction pattern, Structure of simple lattices and X-ray intensities, structure factor and its relation to intensity and electron density, phase problem. Description of the procedure for an X-ray structure analysis, absolute configuration of molecules.

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Suggested Books References:

1. Concepts of Inorganic Photochemistry, A.W. Adamson and P.D. Fleischauer, Wiley.
2. Inorganic Photochemistry, J.Chem. Educ. vol. 60 No. 10, 1983.
3. Progress in Inorganic Chemistry, Vol. 30ed. S.J. Lippard, Wiley.
4. Coordination Chem. Revs. 1981, vol. 39, 121, 1231, 1975, 14, 321.; 1990 97, 313.
5. Photochemistry of Coordination Compounds, V. Balzari and V. Carassiti, Academic Press.
6. Elements in Inorganic Photochemistry, G.J. Ferraudi, Wiley.

MCE 015B: Inorganic Elective II: BIOINORGANIC CHEMISTRY

Course outcome: On completion of this course student will be able to-

CO-1 analyze the structure and function of metal ion containing biomolecules.

CO2 explain principle and mechanism of various cycles involved in energy production and structure and functions of DNA, RNA.

CO3 explain Haem proteins and oxygen uptake structure and function of haemoglobin's, myoglobin, haemocyanins and hemerythrin, model synthetic complexes of iron, cobalt and copper.

CO4 explain Metal deficiency and disease, toxic effects of metals, metals used for diagnosis and chemotherapy. Biological and Chemical nitrogen fixation.

CO5

Unit-I

Metal Ions in Biological Systems

Bulk and trace metals with special reference to Na, K, Mg, Ca, Fe, Cu, Zn, Co, and K^+/Na^+ pump.

Metal Storage and Transport

Ferritin transferrin, and siderophores.

Unit-II

Bioenergetics and ATP Cycle.

DNA polymerisation, glucose storage, metal complexes in transmission of energy; chlorophyll's, photosystem I and photosystem II in cleavage of water.

DNA and RNA

Metal complexes of polynucleotide, nucleosides and nucleic acids (DNA and RNA)

Template temperature stability of DNA.

Unit-III

Transport and Storage of Dioxygen

Haem proteins and oxygen uptake structure and function of haemoglobin's, myoglobin, haemocyanins and hemerythrin, model synthetic complexes of iron, cobalt and copper.

Unit-IV

Metals in Medicine

Metal deficiency and disease, (Iron, Zinc, Copper) toxic effects of metals, metals used for diagnosis and chemotherapy with particular reference the anticancer drugs.

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Nitrogen fixation

Nitrogen in biosphere, nitrogen cycle, nitrification role microorganism, nitrogen fixation in soils, Biological nitrogen fixation, and its mechanism, nitrogenase, Chemical nitrogen fixation

Unit-V

Origin of supramolecular chemistry - "Chemistry beyond the molecules". Concepts and terminology of supramolecular chemistry. Nature and types of supramolecular interactions (Hydrogen bonding, van der Waal interactions, π -stacking, C-H... π interactions etc.). Molecular recognition- Information and complementarity. Different types of receptors with special reference of Crown ethers, cryptates and Calix[4]arene. Molecular self-assembly formation and examples. Supramolecular chemistry of life, application of supramolecular chemistry in drug design. Application in material science-molecular machines.

Suggested Books References:

1. Principals of Bioinorganic Chemistry. S.J. Lppard and J.M. Berg University Science Books.
2. Bioinorganic Chemistry, I Bertini, H.B. Gray. S.J. Lippard and Jon Valentine, University Science Books.
3. Inorganic Biochemistry Vols I and II Ed.
4. Progress in Inorganic Chemistry Vols. 1i 18 Ed J.J. Lippard Wiley.
5. Principles of Bioinorganic Chemistry, S.J. Lippard and J.M. Berg, University Science Books.
6. Bioinorganic Chemistry, 1. Bertini, H.B. Gray, S.J. Lippard and J.S. Valentine, University Science Books.
7. Inorganic biochemistry vol. I and II ed. G.L. Eichhorn, Elsever.
8. Progress in Inorganic Chemistry, Vol 18 and 38 ed J.J. Lippard, Wiley.
9. Supramolecular Chemistry: Concepts and Perspectives; First Edition; J.M. Lehn; VCH Publishers, 2014.
10. Supramolecular Chemistry; Second Edition; J. W. Steed, J. L. Atwood; Wiley, New York, 2009.

MCE016A :Inorganic Elective III: ORGANOTRANSITION METAL CHEMISTRY-I

Course outcome: After the completion of course students will be able to learn about the CO1- types, routes of synthesis, stability and decomposition pathways organo-copper in organic synthesis. CO2- Compounds of Transition Metal-Carbon Multiple Bonds alkylidenes, alkylidyne and their synthesis. CO-3 Compounds of low valent carbenes and carbynes-synthesis CO-4 Transition metal p-Complexes with unsaturated organic molecules, alkenes, alkynes, allyl complexes. CO-5 Transition metal p-Complexes with unsaturated organic molecules, diene, dienyl, arene and trienyl complexes,

Unit-I

Alkyls and Aryls of Transition Metals

Types, routes of synthesis, stability and decomposition pathways organocopper in organic synthesis.

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Unit-II

Compounds of Transition Metal

Carbon Multiple Bonds alkylidenes, alkylidyne, synthesis, nature of bond, structural characteristics, nucleophilic and electrophilic reactions on the ligands, role in organic synthesis.

Unit-III

Compounds of low valent carbenes and carbynes

Synthesis, nature of bond, structural characteristics, nucleophilic and electrophilic reactions on the ligands, role in organic synthesis.

Unit-IV

Transition Metal π -Complexes I

Transition metal π -Complexes with unsaturated organic molecules, alkenes, alkynes, allyl, complexes, preparation, properties, nature of bonding and structural features. Important reactions relating to nucleophilic and electrophilic attack on ligands and to organic synthesis.

Unit-V

Transition Metal π -Complexes II

Transition metal π -Complexes with unsaturated organic molecules, diene, dienyl, arene and trienyl complexes, preparation, properties, nature of bonding and structural features. Important reactions relating to nucleophilic and electrophilic attack on ligands and to organic synthesis

Suggested Books References:

1. Principles and Application of Organotransition Metal Chemistry, J.P. Collman, L.S. Hegsdus, J.R. Norton and R.G. Finke, University Science Books.
2. The Organometallic Chemistry of the Transition Metals, R.H. Crabtree. John Wiley.
3. Metallo-organic Chemistry, A.J. Pearson, Wiley.
4. Organometallic Chemistry, R.C. Mehrotra and A. Singh New Age International

MCE 017A:Spectrophotometric Analysis (Practical)

Preparation (Any Six)

Preparation of selected inorganic compounds and their study by IR, electronic spectra, Mossbauer. ESR and magnetic susceptibility measurements. Handling of air and moisture sensitive compounds involving vacuum lines. Selection can be made from the following :

1. Sodium amide.
2. Synthesis and thermal analysis of group II metal oxalate hydrate.
3. Atomic absorption analysis of Mg and Ca.
4. Preparation of Tin (IV) iodide, Tin (IV) chloride and Tin (II) iodide.
5. Preparation of ammonium hexachlorostannate $(\text{NH}_4)_2 \text{SnCl}_6$ ammonium hexachlorophosphate $(\text{NH}_4)_2 \text{PbCl}_6$.
6. Hexa-bis (4,nitrophenoxy) cyclotriphosphazene.
7. Synthesis of trichlorodiphenylantimony (V) hydrate.
8. Sodium tetrathionate $\text{Na}_2\text{S}_4\text{O}_6$.

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9. Synthesis of metal acetylacetonate .
10. Bromination of $\text{Cr}(\text{acac})_3$.
11. Magnetic moment of $\text{Cu}(\text{acac})_2 \cdot 2\text{H}_2\text{O}$.
12. Cis and Trans $[\text{Co}(\text{en})_2\text{Cl}_2]^+$.
13. Separation of optical isomer of $\text{cis}-[\text{Co}(\text{en})_2\text{Cl}_2]$.
14. Ion exchange separation of oxidation state of vanadium.
15. Preparation and use of Ferrocene.
16. Preparation of copper glycine complex-cis and trans bis (glycinato Copper (II)
17. Preparation of phosphine Ph_3P and its transition metal complexes.
18. Preparation of $[\text{Co}(\text{phenanthroline}-5,6 \text{ quinone})]$.

Spectrophotometric Determinations

1. Manganese/Chromium/Vanadium in steel sample.
2. Nickel/molybdenum/tungsten/vanadium/uranium by extractive spectrophotometric method.
3. Fluoride/nitrite/phosphate.
4. Zirconium-alizarin Red-S complex : Mole-ratio method.
5. Copper-Ethylene diamine complex : Slope-ratio method.
6. Iron-phenanthroline complex : Job's method of continuous variations.

Specialization: Organic Chemistry

MCE 018A: Organic Elective I: ORGANIC SYNTHESIS-I

Course Outcome: After the completion of course, student will be able to

CO1:-Understand the nature of different oxidation process.

CO2:-Understand the various steps involved in the reduction process of organic molecules.

CO3:-Understand the specific reaction mechanism in the process of hydrogenolysis.

CO4:-Understand the basic principle involved in various rearrangement processes.

CO5:- Understand the various steps involved in different rearrangement reactions.

Unit-I

Oxidation

Introduction, Different oxidative processes. Hydrocarbons-alkenes, aromatic rings, saturated C-H groups (activated and unactivated) Alcohols, diols, aldehyde's, ketones, ketals and carboxylic acids. Amines, hydrazines, and sulphides. Oxidations with ruthenium tetroxide, iodobenzene diacetate and thallium. (III) Nitrate.

Unit-II

Reduction-I

Introduction, Different reductive processes. Alkanes, alkenes, alkynes, and aromatic rings. Carbonyl compounds-aldehydes, ketones, acids and their derivatives. Epoxides.

Unit-III

Reduction-II

Introduction, Different reductive processes, Nitro, nitroso, azo and oxime groups. Epoxide, Nitro, Nitroso, azo and oxime groups. Hydrogenolysis.

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Unit-IV

Rearrangements - I

General mechanistic considerations-nature of migration, migratory aptitude, memory effects. A detailed study of the following rearrangements. Pinacol-pinacolone, Wagner-Meerwein.

Unit-V

Rearrangements - II

Demjanov, Benzil-Benzilic acid, Favorskii, Arndt-Eister synthesis, Neber, Beckmann, Hotmann Curtius, Schmidt, Baeyer-Villiger, Shapiro reaction. Schmidt, Baeyer-Villiger. Shapiro reaction

Suggested Books References:

1. Modern Synthetic Reactions, H.O. House, W.A. Benjamin.
2. Some Modern Methods of Organic Synthesis, w. Carruthers, Cambridge Univ. Press.
3. Advanced Organic Chemistry, Reactions Mechanisms and Structure, J. March. John Wiley.
4. Principles of Organic synthesis, R.O.C. Norman and J.M. Coxon, Blackie Academic & Professional.
5. Advanced Organic Chemistry Part B.F.A. Carey and R.J. Sundberg Plenum Press.
6. Rodd's Chemistry of Carbon Compounds. Ed. S. Coffey, Elsevier.

MCE 042A: Organic Elective II: Heterocyclic Chemistry

Course Outcome: After the completion of syllabus, student will be able to learn the

CO-1 Nomenclature patterns of heterocyclic compounds, aromaticity and chemical behaviour

CO-2 Nature, confirmation and stability of non aromatic heterocycles

CO-3 Synthesis and reaction of small ring(3,4,5)membered heterocycles.

CO-4 The synthesis and reaction of benofused and meso-ionic heterocycles.

CO-5 The synthesis and reaction of six membered with one heteroatom and more than one heteroatom

Unit-I

Nomenclature of Heterocycles

Replacement and systematic nomenclature (Hantzsch-Widman system) for monocyclic fused and bridged heterocycles.

Aromatic Heterocycles

General chemical behaviour of aromatic heterocycles, classification (structural type), criteria of aromaticity (bond lengths, ring current and chemical shifts in ¹H NMR-spectra. Empirical resonance energy, delocalization energy and Dewar resonance energy, diamagnetic susceptibility exaltations). Heteroaromatic reactivity and tautomerism in aromatic heterocycles.

Unit-II

Non-aromatic Heterocycles

Strain-bond angle and torsional strains and their consequences in small ring heterocycles.

Conformation of six-membered heterocycles with reference to molecular geometry, barrier to ring inversion, pyramidal inversion and 1,3-diaxial interaction. Stereo-electronic effects anomeric and related effects, Attractive interactions-hydrogen bonding and intermolecular

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nucleophilic electrophilic interactions. Heterocyclic Synthesis. Principles of heterocyclic synthesis involving cyclization reactions and cycloaddition reactions.

Unit-III

Small Ring Heterocycles

Three-membered and four-membered heterocycles-synthesis and reactions of aziridines, oxiranes, thiranes, azetidines, oxetanes and thietanes.

Unit-IV

Benzo-Fused Five-Membered Hetero cycles and Meso Ionic Synthesis and reactions including medicinal applications of benzopyrroles, benzofurans and benzothiophenes Meso-ionic heterocycles: classification, chemistry of some important meso-aionic heterocycles of type-A and B and their applications. Sydnones.

UNIT-V

Six Membered Heterocycles with one heteroatom: synthesis and reactions of pyrilium salts and pyrones and their comparison with pyridinium and thiopyrylium salts and pyridones; synthesis and reactions of quinolizinium and benzopyrylium salts, coumarins and chromones.

With two or more heteroatoms: synthesis and reactions of diazines, triazines, tetrazines and thiazines. Some important macroheterocycles.

Suggested Books References:

1. Heterocyclic Chemistry Vol. 1-3, R.R. Gupta, M. Kumar and V.Gupta, Springer Verlag.
2. The Chemistry of Heterocycles, T. Eicher and S. Hauptmann, Thieme.
3. Heterocyclic chemistry J.A. Joule, K. Mills and g.F. Smith, Chapman and Hall.
4. Heterocyclic Chemistry, T.L. Gilchrist, Longman Scieticif Techinal.
5. Contemporary Hetrocyclic Chemistry, G,.R. Newkome and W.W. Paudler, Wiley-Inter Science.
6. An Introductiion to the Heterocyclic Compounds, R.M. Acheson, Johnwiely.
7. Comprehensive Heterocyclic Chemistry, A.R. Katrizky and C.W. Rees, eds. Pergamon Press.
8. I.L. Finar Organic Chemistry vol 2 (3rd.ed.) Longmans Green & Co.
9. Organic Chemistry by Morrison& Boyd,

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MCE 020B: Organic Elective III: NATURAL PRODUCTS-I

Course outcome: On completion of the course, M.Sc. student will be able to understand:

CO-1 Physical properties, chemical properties, synthesis and uses of terpenoids. It found in various citrus fruits and herbs and is known to have antioxidant properties and is also used in various household products such as detergents and soaps.

CO-2 Classification, nomenclature, isolation and uses of carotenoids. The health benefits of carotenoids generally derive from their vitamin A activity in the body. These benefits include support for the skin, immune system, heart and eyes.

CO-3 Students gain specific knowledge necessary for understanding the structure, isolation and physiological action of alkaloids, their structures, functions, as well as their possible use in human.

CO-4 The general properties of the alkaloids, importance of these compounds to humans. Synthesis and biosynthesis of these natural products are also discussed

CO-5 Nomenclature, basic skeleton, isolation, structure determination and health benefits of steroids

Unit - I**Terpenoids**

Classification, nomenclature, occurrence, isolation, general methods of structure determination, isoprene and biogenic isoprene rules. Structure and synthesis of the following representative molecules: Citral, Geraniol, α -Terpeneol, Zingiberene, Santonin, abietic acid, biogenesis of terpenes.

Unit-II**Carotenoids**

Introduction, nomenclature, occurrence, isolation, general methods of structure determination, structure and synthesis of β -Carotene, Vitamin-A, Capsorubin, Kuhn-Roth methyl side-chain determination.

Unit-III Alkaloids-I

Definition, nomenclature and physiological action, occurrence, isolation, general methods of structure elucidation, degradation (Hofmann's exhaustive, Emde and Von Braun's method), classification based on nitrogen heterocyclic ring, structure and synthesis of D-ephedrin, Coniine.

Unit-IV**Alkaloids-II**

Structure, stereochemistry, synthesis and biosynthesis of the following: Nicotine, Atropine, Cocaine, Quinine and Morphine.

Unit-V**Steroids**

Occurrence, nomenclature, Diel's hydrocarbon, isolation, structure determination and synthesis of Cholesterol, Bile acids, steroidal hormones (Androsterone, Testosterone, Oestrone), Progesterone, Aldosterone, Biosynthesis of Steroids.

Suggested Books References:

1. Natural Products : Chemistry and Biological Significance, J. Mann, R.S. Davidson, J.B. Hobbs, D.V. Banthorpe and J.B. Harborne, Longman, Essex.
2. Organic Chemistry : Vol. 2 I.L. Finar, ELBS
3. Stereoselective Synthesis : A Practical Approach, M. Norrgradi, VCH.
4. Rodd's Chemistry of Carbon Compounds, Ed. S. Coffey, Elsevier.

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5. Chemistry, Biological and Pharmacological Properties of Medicinal Plants from the Americas, Ed. Kurt Hostettmann, M.P. Gupta and A. Marston, Harwood Academic Publishers.
6. Introduction to Flavonoids, B.A. Bohm, Harwood Academic Publishers.
7. New Trends in Natural Product chemistry, Ata-ur-Rahman and M.L. Choudhary, Harwood Academic Publishers.
8. Insecticides of Natural Origin, Sukh Dev, Harwood Academic Publishers

MCE 021A: Multi-step Synthesis (Practical)

Qualitative Analysis

Separation, purification and identification of the components of a mixture of three organic compounds (three solids or two liquids and one solid or two solids and one liquid), using TLC for checking the purity of the separated compounds, chemical analysis, IR, PMR and Mass spectral data.

Multi-step Synthesis of Organic Compounds

The exercise should illustrate the use of organic reagents and may involve purification of the products by chromatographic techniques.

1. Photochemical reaction Benzophenone \rightarrow Benzopinacol \rightarrow Benzpinacolone
2. Beckmann rearrangement : Benzanilide from benzene, Benzene \rightarrow Benzophenone \rightarrow Benzophenone oxime \rightarrow Benzanilide
3. Benzilic acid rearrangement : Benzilic acid from benzoin Benzoin \rightarrow Benzil \rightarrow Benzilic acid Synthesis of heterocyclic compounds
4. Skraup synthesis : Preparation of quinoline from aniline
5. Fisher Indole synthesis : Preparation of 2-phenylindole from phenylhydrazine.
6. Enzymatic synthesis Enzymatic synthesis
7. Enzymatic reduction : reduction of ethyl acetoacetate using Baker's yeast to yield enantiomeric excess of S (+) ethyl-3-hydroxybutanoate and determine its optical purity.
8. Biosynthesis of ethanol from sucrose.
9. Synthesis using microwave Alkylation of diethyl malonate with benzyl chloride.
10. Synthesis using phase transfer catalyst. Alkylation of diethyl malonate or ethyl acetoacetate with an alkylhalide.

Paper Chromatography

Separation and identification of the sugars present in the given mixture of glucose, fructose and sucrose by paper chromatography and determination of R_f values.

Spectroscopy

Identification of organic compounds by the analysis of their spectral data (UV, IR, PMR, C^{13} NMR & MS) Spectrophotometric (UV/VIS) Estimations -

1. Amino acids
2. Proteins
3. Carbohydrates
4. Cholesterol
5. Ascorbic acid
6. Aspirin
7. Caffeine

Books Suggested

1. Inorganic Experiments, J. Derek Woolings, VCH.

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2. Microscale Inorganic Chemistry, Z. Szafran, R.M. Pike and M.M. Singh, Wiley.
3. Practical Inorganic Chemistry, G. Marr and B. W. Rockett, Van Nostrand.
4. The systematic Identification of Organic Compounds, R.L. Shriner and D.Y. curlin.

Specialization: Physical Chemistry

MCE 022A: PHYSICAL ELECTIVE I: ELECTROANALYTICAL TECHNIQUES

Course outcome: On completion of the course, M.Sc. student will be able to understand:

- CO-1 Introductory idea of analytical methods and laboratory operations.
 CO-2 Errors and evaluation of statistical data and methods of reporting analytical data
 CO-3 Conductometric titrations and measurements.
 CO-4 Potentiometric methods, pH determination by instruments and its applications
 CO-5 principle and applications of colorimetry

Unit I

Introduction

Role of analytical chemistry Classification of analytical methods classical and instrumental. Types of instrumental analysis. Selecting an analytical method. Neatness and cleanliness. laboratory operations and practices. Analytical balance. Techniques of weighing, errors. Volumetric glassware cleaning and calibration of glassware. Cleaning and Calibration of glassware. Sample preparation-dissolution and decompositions.

Unit II

Errors and Evaluation (Statistical Analysis)

Definition of terms in mean and median. Precision-standard deviation, relative standard deviation. Accuracy-absolute error, relative error. Types of error in experimental data determinate (systematic), indeterminate (or random) and gross. Sources of error and the effects upon the analytical results. Methods for reporting analytical data. Statistical evaluation of data-indeterminate errors. The uses of statistics.

Unit III

Conductometry

Important laws, definitions, relations, effect of dilution on conductivity, measurement of conductivity, types of conductometric titrations, its applications and limitations.

Unit IV

Potentiometry

Principle instrumentation, types of potentiometric titrations and its applications, pH measurements, determination of pH, ion selective electrodes, instrumentation and its applications

Unit V

Coulometry

Introduction, principle, experimental details of coulometry at constant current and constant potential, titrational applications.

Suggested Books References:

1. Principles of Instrumental analysis D.A. Skoog and J.L. Loary, W.B. Saunders.
2. Principles of Instrumental Analysis D.A. Skoog W.B. Saunders.
3. Handbook of Instrumental Techniques for Analytical Chemistry, F. Settle, Prentice Hall

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MCE 023A: PHYSICAL ELECTIVE II : ELECTROCHEMISTRY-I

Course outcome: On completion of the course, student will be able to understand about the

CO-1 Electrochemical batteries

CO-2 role of electrochemical reactions in biological processes.

CO-3 details of the process of corrosion.

CO-4 corrosion inhibition methods

CO-5 Kinetics of electrode process

Unit I

Electrochemical Energy Storage

Properties of Electrochemical energy storers : Measure of battery performance, Charging and discharging of a battery, Storage Density, Energy Density. Classical Batteries : (i) Lead Acid (ii) Nickel-Cadmium, (iii) Zinc manganese dioxide. Modern Batteries : (i) Zinc-Air (ii) Nickel-Metal Hydride, (iii) Lithium Battery, Future Electricity storers : Storage in (i) Hydrogen, (ii) Alkali Metals, (iii) Non aqueous solutions.

Unit II

Bioelectrochemistry

Membrane Potentials, Simplistic theory, Modern theory, Electrical conductance in biological organism: Electronic, Protonic electrochemical mechanism of nervous systems, enzymes as electrodes.

Unit III

Corrosion and Stability of Metals :

Civilization and Surface mechanism of the corrosion of the metals; Thermodynamics and the stability of metals, Potential -pH (or Pourbaix) Diagrams; uses and abuses, Corrosion current and corrosion potential -Evans diagrams. Measurement of corrosion rate : (i) Weight Loss method, (ii) Electrochemical Method.

Unit IV

Inhibiting Corrosion

Cathodic and Anodic Protection. (i) Inhibition by addition of substrates to the electrolyte environment, (ii) by changing the corroding method from external source, anodic Protection, Organic inhibitors, The fuller Story Green inhibitors.

Passivation

Structure of Passivation films, Mechanism of Passivation, Spontaneous Passivation Nature's method for stabilizing surfaces.

Unit V

Kinetic of Electrode Process :

Essentials of Electrode reaction. Current Density, Overpotential, Tafel Equation, Butler Volmer equation. Standard rate constant (K_0) and Transfer coefficient (α), Exchange Current.

Irreversible Electrode processes

Criteria of irreversibility, information from irreversible wave. Methods of determining kinetic parameters for quasi-reversible and irreversible waves, Koutecky's methods, Meites Israel Method, Gellings method

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Suggested Books References:

1. Modern Electrochemistry Vol. I, Ila, Vol. IIB JOM Bockris and A.K.N. Reddy, Plenum Publication, New York.
2. Polarographic Techniques by L. Meites, Interscience.
3. "Fuel Cells : Thjeir electrochemistry". McGraw Hill Book Company, New York.
4. Modern Polarographic Methods by A.M. Bond, Marcell Dekker.
5. Polarography and allied techniques by K. Zutshi, New age International publicatin. New Delhi.
6. "Electroanalytical Chemistry by Basil H. Vessor & Galen W. ; Wiley Interscience.
7. Electroanalytical Chemistry by Basil H. Vessor & alen w. ; Wiley Interscience.
8. Topics in pure and Applied Chemistry, Ed. S. K. Rangrajan, SAEST Publication, Karaikudi (India)

MCE 024A: PHYSICAL – ELECTIVE III :CHEMICAL KINETICS I

Course outcome: On completion of the course, M.Sc. student will be able to understand:

CO-1 kinetics of oscillatory reactions

CO-2 Kinetics of enzyme inhibition reactions

CO-3 Adsorption-desorption kinetics and importance of Industrial catalysts

CO-4 statistical mechanics and transition state theory, applications in calculation of the second order rare constant for reactions.

CO-5 mechanism of metal ion catalysis

Unit I

Oscillatory Reactions

Autocatalysis and oscillatory reactions, Kinetics and mechanism of Belousov-Zhabotinski (B-Z) reactions.

Unit II

Enzymes and Inhibitions

Kinetics of one enzymes-Two substrate systems and their experimental characteristics, Kinetics of enzyme inhibited reactions, Enzyme inhibitors and their experimetnal characteristics.

Unit III

Dynamics of Gas-surface Reactions

Adsorption/desorption kinetics and transition state theory. Dissociative adsorption and precursor state. Mechanism of Langmur's adsorption of the oxidation of carbon monoxide to carbon dioxide. True and apparent activation energies. Industrial imporance of heterogeneous catalysis.

Unit IV

Transition State

A brief aspect of statistical mechanics and transition state theory. Application in calculation of the second order rare constant for reactions with collision for (1) atom + atom, (2) atom + molecule (linear), (3) atom + non linear molecule, (4) linear and linear molecule, (5) linear molecule + non linear molecule reactions. Static solvent effects and thermodynamics formulations. Adiabatic electron transfer reactions, energy surfaces.

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Unit V

Metal ion catalysis

Kinetics and mechanism of following reaction-

- When reaction rate is independent of one of the reactants in presence of metal ion catalyst
 - When reaction rate is retarded of one of the products in the presence of metal ion catalyst.
 - When metal ion catalysis indicates an intermediate complex.
- (b)(i). Cyclodextrines and their mode of catalysis, a case study.

Suggested Books References:

1. Progress in Inorganic Chemistry, Vol. 30 1967.
2. R. Lumry and R.W. Raymond, Electron Transfer Reactions, Interscience.
3. N.L. Bender, Mechanism of Homogeneous Catalysis from protein to protein, Wiley.
4. A.G. Sykes, Kinetics of Inorganic reactins, Pergamon.
5. S.W. Benson, Mechanism of Inorganic Reactions, Academic Press.
6. Physical Chemistry Vol. 2, Ed. Prof Ya Grasimov, Mir publisher.
7. Basolo and Pearson, Inorganic Reactino Mechaims, Wiley.
8. H. Taube, Electron Transfer Reactions, Oxford Press.

MCE 025A: Thermodynamical Studies (Practical)

1. Determination of partial molar volume of solute (e.g. KCl) and solvent in a binary mixture.
2. Determination of the temperature dependence of the solubility of a compound in two solvents having similar intramolecular in tetrations (benzoic acid in water and in DMSO water mixture and calculate the partial molar heat of solution.
3. Determination of Pka of an indicator (e.g. methyl red) in (a) aqueous and (b) micellar media.
4. Determination of stoichiometry and stability constant of Ferricisothiocyanate complex ion in solution.
5. Determination of rate constant of alkaline bleaching of Malachite green and effect of ionic strength on the rate of reaction.
6. Verify Beer,s law for solution of KMnO_4 and determine concentration of given aqueous solution of unknown concentration of this salt.
7. Determine the solubility and solubility product of a sparingly soluble salt conductometrically.
8. Determine the dissociation constant of a weak acid conductometrically and verify ostwalds dilution law.
9. Study the hydrolysis of methyl acetate catalysed by HCl solution and equinormal solution of urea hydrochloride and determines the degree of hydrolysis of the salt.
10. Study saponification of ethyl acetate conductometrically.
11. Oscillatory reaction(demonstration) and note down the time for damping of oscillation.
12. Study the reaction rate of decomposition of H_2O_2 Kinetically in presence of iodide in acid solution.

Books Suggested

- i. Inorganic Experimens, J. Derek Woolings, VCH.
- ii. Microscale Inorganic Chemistry, Z. Szafran, R.M. Pike and M.M. Singh, Wiley.

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- iii. Practical Inorganic Chemistry, G. Marr and B. W. Rockett, Van Nostrand.
- iv. The systematic Identification of Organic Compounds, R.L. Shriner and D.Y. curlin.

Semester IV

Specialization: Inorganic Chemistry

MCE 027A: Inorganic Elective I: ORGANOTRANSITION METAL CHEMISTRY-II

Course outcome: After the completion of course

- CO-1 Students will be able to understand the transition metal compounds with bonds to hydrogen .
- CO-2 Students will be able to apply and analyze the basic knowledge of stoichiometric reactions for catalysis.
- CO-3 Students will be able to describe the basic concept of catalytic reactions involving carbon monoxide.
- CO-4 Students will be able to explain reactions involving activation of C-H bond.
- CO-5 Students will be able to understand fluxional Organometallic Compounds and their properties.

Unit-I

Transition metal compounds with bonds to hydrogen
Transition metal compounds with bonds to hydrogen.

Unit-II

Homogeneous Catalysis

Stoichiometric reactions for catalysis, homogeneous catalytic hydrogenation, Zeigler-Natta polymerization of olefins,

Unit-III

Reactions of CO

Catalytic reactions involving carbon monoxide such as hydrocarbonylation of olefins (oxoreaction), explanation reactions,

Unit-IV

Activation of C-H bond

Reactions involving activation of C-H bond

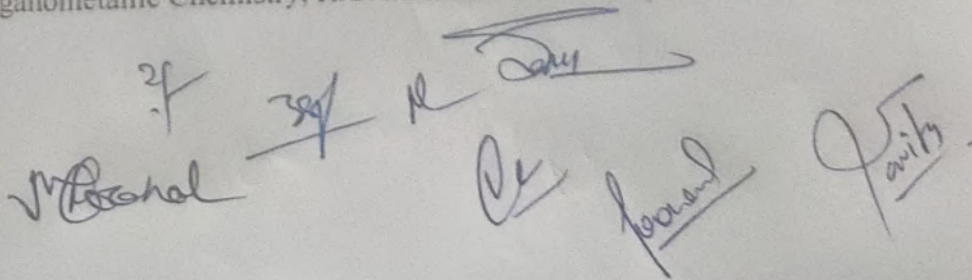
Unit-V

Fluxional Organometallic Compounds

Flexionality and dynamic equilibrium in compounds such as η^2 olefine, η^3 -allyl and dienyl complexes.

Suggested Books References:

1. Principles and Application of Organotransition Metal Chemistry, J.P. Collman, L.S. Hegsdus, J.R. Norton and R.G. Finke, University Science Books.
2. The Organometallic Chemistry of the Transition Metals, R.H. Crabtree. John Wiley.
3. Metallo-organic Chemistry, A.J. Pearson, Wiley.
4. Organometallic Chemistry, R.C. Mehrotra and A. Singh New Age International.



MCE 028A: Inorganic Elective II: INORGANIC POLYMERS

Course Outcome: After the completion of this course

- CO-1 Students will be able to understand the basic concept of polymers.
- CO-2 Students will be able to explain basic knowledge of polymer characterization and poly dispersion concept.
- CO-3 Students will be able to describe the structure, properties and applications of polymers based on boron.
- CO-4 Students will be able to explain the structure, properties and applications of polymers based on silicon.
- CO-5 Students will be able to explain the structure, properties and applications of polymers based on phosphorous.

Unit-1

Basics

Importance of polymers. Basic concepts : Monomers, repeat units, degree of polymerization
Linear, branched and network polymers. Classification of polymers. Polymerization :
condensation, addition/radical chain-ionic and co-ordination and copolymerization.
Polymerization conditions and polymer reactins. Polymerization in homogeneous and
heterogeneous systems.

Unit-II

Polymer Characterization

Polydispersion-average molecular weight concept. Number, weight and viscosity average
molecular weights. Polydispersity an molecular weight distribution.

Unit-III

Polymers of Boron

Structure, Properties and Applications of Polymers based on boron-borazines, boranes and
carboranes.

Unit-IV

Polymes of silicon

Structure, Properties and Applications of Polymers based on Silicon, silicone's polymetalloxanes
and polymetallosiloxanes, silazanes.

Unit-V

Polymers of Phosphorous and sulphur

Structure, Properties and Application of-

- i. Polymers based on Phosphorous-Phosphazenes, Polyphosphates
- ii. Polymers based on Sulphur -Tetrasulphur tetranitride and related compounds.

Suggested Books References:

1. Inorganic Chemistry, J.E. Huheey, Harper Row.
2. Developments in Inorganic polymer Chemistry, M.F. Lappert and G.J. Leigh.
3. Inorganic polymers- N.H> Ray.
4. Inorganic polymers, Graham and Stone.
5. Inorganic Rings and Cages : D.A. Armitage.

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6. Textbook of Polymers Science, F.W. Billmeyer Jr. Wiley.
7. Contemporary Polymer Chemistry, H.R. Alcock and F.W. Lambe, Prentice Hall

MCE 029B: Inorganic Elective III: MINERAL BASED INDUSTRIAL CHEMISTRY

Course Outcome: After the completion of this course:

- CO-1 Students will be able to understand general principles applied in studying an industry and manufacture of iron, steels etc.
- CO-2 Students will be able to explain classification of cement and manufacture of portland cement.
- CO-3 Students will be able to describe the classification of ceramics and basic raw materials.
- CO-4 Students will be able to explain the solid industrial poisons and their classification.
- CO-5 Students will be able to explain the liquid and gaseous industrial poisons and their classification.

Unit-I

INDUSTRIAL CHEMISTRY

Ferrous and non-ferrous industries-quality control methods, general principles applied in studying an industry –manufacture of iron, steels metallurgy of gold and silver.

Unit-II

CEMENT

Classification of cement, manufacture of Portland cement –setting and hardening of cement, chemical constitution of Portland cement and their characteristics – special cement and their characteristics –special cements and their uses.

Cermics

Unit-III

Ceramics

Classification of ceramics, basic raw materials-application of colours to pottery porcelain and china ware-manufacture, glass-raw materials, manufacture of special glass-optical, borosilicate, flint and coloured glass.

Unit-IV

Main group elements and their compounds: Allotropy, synthesis, structure and bonding, industrial importance of the compounds.

Unit-V

Classification of pollutants : Their sources, Sewage water treatment:, waste water treatment – domestic and industrial.

Suggested Books References:

1. Chemical Process Industries; N.D. Shreeve.
2. Applied Chemistry for Engineer; Diamont.
3. Chemistry of engineering materials; Jain & Jain
4. Engineering chemistry; B.K. Sharma.

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MCE 030A: Flame Photometric and Flame Photometric Determination (Practical)

Flame Photometric Determinations

1. Sodium.
2. Potassium
3. Sodium and potassium when present together
4. Lithium
5. Calcium
6. Barium
7. strontium.
8. Cadmium
9. Magnesium in tap water.

Quantitative determinations of a two component mixture

One Volumetrically and one gravimetrically

1. Cu^{+2} , Ni^{+2}

Quantitative determinations of a three component mixture :

One Volumetrically and two gravimetrically

1. Cu^{+2} , Ni^{+2} , Zn^{+2}
2. Cu^{+2} , Ni^{+2} , Ng^{+2}

Specialization: Organic Chemistry

MCE 031A: Organic Elective I: Disconnection Approach

Course Outcome: On completion of the course, M.Sc. student will be able to understand:

- CO-1** Synthons and synthetic equivalents, disconnection approach, chemo selectivity, Order of Reactions etc.
- CO-2** Principle of protection of alcohol, amine, carbonyl and carboxyl groups, Alcohols and carbonyl compounds, regioselectivity, alkene synthesis, use of acetylenes and aliphatic Nitro compounds in organic synthesis.
- CO-3** Diels-Alder Reaction, 1,3-difunctionalised compounds, a-b- unsaturated carbonyl compounds, control in carbonyl condensations, 1,5-difunctionalised compounds. Micheal addition and Robinson annelation.
- CO-4** Retrosynthesis of Saturated heterocycles, synthesis of 3,4,5 and 6 membered rings. aromatic heterocycles in organic synthesis. General strategy and stereoselectivity, Cyclisation and insertion reaction rearrangement in synthesis.
- CO-5** Retrosynthesis in Photocycloaddition and use of ketenes, Pericyclic rearrangement and special methods, carbonyl condensation, Diels -Alder reaction and reduction of aromatic compounds as a tool for retrosynthetic analysis.

Unit-I

Disconnection Approach

An introduction to synthons and synthetic equivalents. Disconnection approach, functional group inter-conversions, the importance of the order of events in organic synthesis, one group C-X and two group C-X disconnections, Chemoselectivity, reversal of polarity, cyclisation reaction, amine synthesis.

Unit-II

Protecting Groups

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

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One Group C-C Disconnections

Alcohols and carbonyl compounds, regioselectivity, alkene synthesis, use of acetylenes and aliphatic Nitro compounds in organic synthesis.

Unit-III

Two Group C-C Disconnections

Diels-Alder Reaction, 1,3-difunctionalised compounds, α,β -unsaturated carbonyl compounds, control in carbonyl condensations, 1,5-difunctionalised compounds. Micheal addition and Robinson annelation.

Unit-IV

Ring Synthesis-I

Saturated heterocycles, synthesis of 3,4,5 and 6 membered rings. aromatic heterocycles in organic synthesis. General strategy and stereoselectivity, Cyclisation and insertion reaction, rearrangement in synthesis,

Unit-V

Ring Synthesis-II

Photocycloaddition and use of ketenes, Pericyclic rearrangement and special methods, carbonyl condensation, Diels-Alder reaction and reduction of aromatic compounds.

Suggested Books References:

1. Designing Organic Synthesis, S. Warren. Wiley.
2. Organic Synthesis-Concept, Methods and Starting Materials, J. Fuhrhop.
3. Some Modern Methods of Organic Synthesis. W. Carruthers, Cambridge Univ. Press.
4. Modern Synthetic Reactions H.O. House, W.A Benjamin.
5. Advanced Organic Chemistry : Reactions, Mechanisms and Structure, J. March. Wiley.
6. Principles, of Organic Chemistry Part B. F.A. Carey and R.J. Sundberg, Plenum Press.

Organic Elective-II: MCE043A Advanced Organic Spectroscopy

Course Outcomes: After the completion of the course, student will be able to-

- CO1 Understand the advanced Proton magnetic resonance spectroscopy, complex splitting patterns etc.
- CO2 Understand the Principles ^{13}C spectroscopy, their applications in structure determination and working method of Instrument and two dimensional spectroscopy, 2DNMR inadequate - COSY, NOESY, HETCOR.
- CO3 Understand the mass spectrometry in detail.
- CO4 Understand the UV spectra of heterocyclic, azulenes and acetylinic compounds, optical rotation, optical rotatory dispersion (ORD), circular dichorism (CD), octant rule and axial halo ketone rule.
- CO5 apply the knowledge of various spectroscopic techniques in structure identification of organic compounds.

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UNIT-I

Proton magnetic resonance spectroscopy

Nuclear properties, Pulse techniques, Fourier Transform technique and its advantages, complex splitting patterns (AX, AB, AB_X, AM_X, ABC, AM₃, A₂X₂, A₂X₃), coupling constant [germinal, vicinal, long range (allylic, homoallylic), coupling through space].

Hindered rotation, Karplus equation and curve variation of coupling constant with dihedral angle, simplification of complex spectra: nuclear magnetic double resonance, contact shift reagents, variable temperature dynamic NMR spectroscopy.

Effect of quadrupolar nuclei (10B) on the ¹H NMR spectra, Satellite spectra -examples for different spin systems -Systems with chemical exchange -study of fluxional behavior of molecules.

A brief introduction of compounds carrying NMR active nuclei like N¹⁵, F¹⁹, P³¹.

UNIT- II

¹³C NMR spectroscopy ¹³C NMR spectroscopy: Basic principles Carbon- 13 NMR spectroscopy, chemical shift (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbon). Two dimension NMR spectroscopy.

proton (¹H) coupled ¹³C NMR spectrum, off-resonance and noise decoupled ¹³C NMR spectrum, DEPT . 2DNMR inadequate – COSY, NOESY, HETCOR.

Unit-III

Mass Spectrometry

Introduction, ionization methods EI, CI, FD and FAB, Fragmentation: basic fragmentation types and rules, factors affecting fragmentation, ion analysis, ion abundance, Mass spectral fragmentation of organic compounds (hydrocarbons, alcohols, ethers, ketones, aldehydes, carboxylic acids, amines, nitriles, nitro and halogenated compounds), common functional groups, molecular ion peak, meta stable peak. Mc-Lafferty rearrangement. Nitrogen rule, HRMS.

Unit-IV

UV-Visible spectroscopy and ORD

Determination of configuration of E/Z isomer, steric effect, UV spectra of heterocyclic, azulenes and acetylenic compounds, optical rotation, optical rotatory dispersion (ORD), circular dichorism (CD), octant rule and axial halo ketone rule.

Unit-V

Structure Elucidation of complex organic molecules

Structure elucidation of organic compounds by combined applications of UV, IR, NMR and mass spectrometry

Suggested Books References:

1. Spectrometric Identification of Organic Compounds; Sixth Edition; R.M. Silverstein and F.X. Webster; John Wiley and Sons, 2002.
2. Organic Spectroscopy; Third Edition; W. Kemp; Palgrave Publisher Ltd., New York, 2004.
3. Spectroscopic Methods in Organic Chemistry; Sixth Edition; D. H. Williams and I. Fleming; Tata McGraw Hill Publishing Company Ltd, New Delhi, 2002.
4. Spectral Analysis of Organic Compounds; Second Edition; C.J. Creswell and M.M. Campbell; Burgess Publishing Company, Great Britain, 1972.

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MCF 033C: Organic Elective III: NATURAL PRODUCTS-II

Course Outcome: After the completion of this course

- CO-1 Students will be able to understand primary function of pigments in plants and general methods of structure determination.
- CO-2 Students will be able to describe biosynthesis of plant pigments and gain knowledge about Acetate pathway and Shikimic acid pathway.
- CO-3 Students will be able to describe the Structure, synthesis and binding of Haemoglobin and Structure, synthesis of light absorbing pigment Chlorophyll.
- CO-4 Students will be able to explain isolation, nomenclature, classification, biogenesis and physiological effects of Prostaglandins.
- CO-5 Students will be able to understand synthesis and structure elucidation of Pyrethroids and Rotenones. Student will also be able to understand the concepts of medicinal chemistry.

Unit-I

Plant Pigments-I

Occurrence, nomenclature and general methods of structure determination, structure and synthesis of cyanidin chloride, pelargonidin chloride, delphinidin and hirsutidin chlorides.

Unit-II

Plant Pigments-II

Occurrence, nomenclature, structure and synthesis of flavonol (3-hydroxy flavone), quercetin, isoflavone, daidzein, butin and aureusin, butein, Aureusin, Biosynthesis of flavonoids.

Unit-III

Prophyrins

Haemoglobin, degradation products of haemoglobin and synthesis of haemin, porphyrins, spectral properties, structure elucidation and synthesis of Chlorophyll.

Unit-IV

prostaglandin

Occurrence, nomenclature, classification, biogenesis and physiological effects. Synthesis of PGE2 and PGF2a.

Unit-V

Pyrethroids and Rotenones

Synthesis and reactions of Pyrethroids and Rotenones. (For structure elucidation, emphasis is to be placed on the use of spectral parameters wherever possible).

Medicinal Chemistry:

Drugs and their Classification, Drug-target interactions, Therapeutic action of a new important

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class of drugs(antacids,antihistamines),neurologically active drugs,(tranquilizers,analgesics), antimicrobials(antibiotics,antiseptics & disinfectants), anticancer drugs;Taxol, Artemisinin antifertility drugs,artificial sweetening agents(sucralose rotenoid) and food preservatives. New development in Drug research.Drug designing.

Suggested Books References:

1. Natural Products : Chemistry and Biological Significance, J. Mann, R.S. Davidson, J.B. Hobbs, D.V. Banthorpe and J.B. Harborne, Longman, Essex.
2. Organic Chemistry : Vol. 2 I.L. Finar, ELBS
3. Stereoselective Synthesis : A Practical Approach, M. Norgradi, VCH.
4. Rodd's Chemistry of Carbon Compounds, Ed. S. Coffey, Elsevier.
5. Chemistry, Biological and Pharmacological Properties of Medicinal Plants from the Americas, Ed. Kurt Hostettmann, M.P. Gupta and A. Marston. Harwood Academic Publishers.
6. Introduction to Flavonoids, B.A. Bohm. Harwood Academic Publishers.
7. New Trends in Natural Product chemistry, Ata-ur-Rahman and M.L. Choudhary, Harwood Academic Publishers.

MCE 034A: Chromatography and Spectroscopy (Practical)

Thin Layer Chromatography

1. To separate the mixture of Methyl Orange and Methylene Blue by using cyclohexane and ethyl acetate(8.5:1.5) as solvent system.
2. To Prepare and separate 2,4-dinitro Phenylhydrazone of acetone, 2-butanone, hexane-2-one and hexane-3-one using toluene and petroleum ether(40:60).

Paper Chromatography

3. To separate the mixture of phenylalanine and glycine. Alanine and aspartic acid. Leucine and glutamic acid. Spray reagent - Ninhydrin.
4. To separate the mixture of D,L-alanine, glycine and L-leucine using n-butanol : acetic acid : water(4:1:5). Spray reagent- Ninhydrin.
5. To separate monosaccharides - a mixture of D - galactose and D-fructose using n-butanol : acetone: water (4:1:5). Spray reagent - aniline hydrogen phthalate.
6. To Separate and identify sugars present in the given mixture of glucose, fructose and sucrose by paper chromatography and determination of R_f values.

Spectroscopy

Identification of organic compounds by the analysis of their spectral data (UV, IR, PMR, CMR & MS) Spectrophotometric (UV/VIS) Estimations-

- i. Amino acids
- ii. Proteins
- iii. Carbohydrates
- iv. Cholesterol
- v. Ascorbic acid
- vi. Aspirin
- vii. Caffeine

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Specialization: Physical Chemistry

MCE 035A: PHYSICAL ELECTIVE I: CHEMICAL ANALYSIS

Course Outcome: After the completion of this course

CO-1 Students will be able to understand Food analysis, use of HPLC and TLC in food adulteration etc

CO-2 Students will be able to analyse soil characteristics and quality

CO-3 Students will be able to perform the analysis of solid, liquid and gaseous fuels.

CO-4 Students will be able to perform the analysis of water, various parameters and impurities present in water.

CO-5 Students will be able to understand clinical analysis and drug analysis by various physical methods.

Unit I

Food analysis

Moisture, ash, crude protein, fat crude fibre, carbohydrates, calcium, potassium, sodium and phosphate. Food adulteration-common adulterants in food, contamination of foods stuffs. Microscopic examination of foods for adulterants. Pesticide analysis in food products. Extraction and purification of sample. HPLC. Gas chromatography for organophosphates. Thin-layer chromatography for identification of chlorinated pesticides in food products.

Unit II

Analysis of soil

Analysis of Soil, moisture pH total nitrogen, phosphorus, silica, lime, manesia, manganese, sulphur and alkali salts.

Unit III

Analysis of Fuel

Fuel analysis : liquid and gas. Ultimate and proximate analysis-heating values-grading of coal. Liquid fuels-flash point, aniline point, octane number and carbon residue. Gaseous fuels-produced gas and water gas-calorific value

Unit IV

Analysis of Water

Objectives of analysis-parameter for analysis-colour, turbidity, total solids, conductivity, acidity, alkalinity, hardness, chloride, sulphate, fluoride, silica, phosphates and different forms of nitrogen, Heavy metal pollution-public health significance of cadmium, chromium, copper, lead, zinc, manganese, mercury and arsenic.

Unit V

Clinical Chemistry

Composition of blood-collection and preservation of samples. Clinical analysis. Serum electrolytes, blood glucose, blood urea nitrogen, uric acid, albumin, globulins, barbiturates, acid

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and alkaline phosphates. Immuno assay : principles of radio immunoassay (RIA) and applications. The blood gas analysis trace elements in the body.

Drug analysis

Narcotics and dangerous drug. Classification of drugs. Screening by gas and thin-layer chromatography and spectrophotometric measurements.

Suggested Books References:

1. Analytical Chemistry, G.D. Christian, J.Wiley.
2. Fundamentals of analytical Chemistry. D.A. Skoog. D.M. West and F.J. Hooler, W.B. Saunders.
3. Analytical Chemistry-Principles. J.H. Kennedy. W.B. Saunders.
4. Analytical Chemistry-Principles and Techniques. LG. Hargis. Prentice Hall.
5. Principles of Instrumental analysis D.A. Skoog and J.L. Loary, W.B. Saunders.
6. Principles of Instrumental Analysis D.A. Skoog W.B. Saunders.
7. Quantitative Analysis, R.A. Day, Jr. and A.L. Underwood, Prentice Hall.
8. Environmental Solution, S.M. Khopkar, Wiley Eastern.
9. Basic Concepts of Analysis Chemistry, S.M. Khopkar, Wiley Eastern.
10. Handbook of Instrumental Techniques for Analytical Chemistry, Settle, Prentice Hall.

MCE 036A : PHYSICAL ELECTIVE II: ELECTRO CHEMISTRY-II

Course Outcome: After the completion of this course

CO-1 Students will be able to understand the formation and working of fuel cells

CO-2 Students will be able to understand the electrocatalysis in simple redox reactions and biological systems. CO-3 Students will be able to understand the principles and applications of voltammetry. CO-4 Students will be able to understand the types of electro organic reaction and their applications in sewage water treatment. CO-5 Students will be able to understand controlled current techniques.

Unit I

Fuel cell

Electrochemical Generators (Fuel Cells) : Hydrogen oxygen cells, Hydrogen Air cell, Hydrocarbon air cell, Alkaline fuel cell, Phosphoric acid fuel cell, direct NaOH fuel cells, applications of fuel cells.

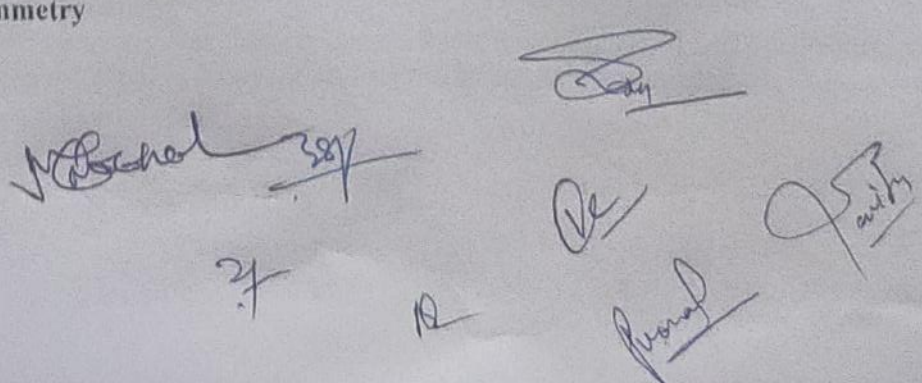
Unit II

Electrocatalysis

Chemical catalysts and Electrochemical catalysts with special reference to porphyrins, oxides of rare earths. Electrocatalysis in simple redox reactions, in reaction involving adsorbed species. Influence of various parameters.

Unit III

Voltammetry



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General principle and applications, linear sweep voltammetry (LSV), cyclic voltammetry (CV), square wave voltammetry, stripping voltammetry, cathodic and anodic adsorptive stripping voltammetry (CAAdSV and AAdSV).

Unit IV

Electro-organic synthesis

Types of electro organic reaction, constant current and constant potential electrolysis, cell design, effect of variable, nature of medium, nature of electrode materials, over voltage, effect of redox couple, application of sewage waste water treatment.

Unit V

Controlled Current Techniques

Introduction, general theory, Sand equation, programmed current chronopotentiometry, Quasireversible waves, reversal techniques, galvanostatic double pulse method.

Suggested Books & References:

1. Electrochemical methods by Allen J. Bard and Larry R. Faulkner, John Wiley. Pub.
2. Electrochemistry by Carl H. Hamann, Andrew Hammett and Wolfgang Vielstich.
3. Modern Polarographic Methods by H. Vossler & Galen W. Wiley Interscience.
4. Topics in pure and applied chemistry Ed. S.K. Rangrajan SAEST Pub., Karaikudi, (India).
5. Techniques of electro-organic synthesis Part I, II & III by N.L. Weinberg John Wiley Pub.

MCE 037A: PHYSICAL ELECTIVE III : CHEMICAL KINETICS-II

Course Outcome: After the completion of this course

- CO-1 Students will be able to understand the kinetics and mechanism of micelle catalyzed reactions
- CO-2 Students will be able to understand the radiation chemistry and photochemistry. Kinetics and mechanism of photochemical and photosensitized reactions, electron transfer reactions.
- CO-3 Students will be able to understand the kinetics and mechanism of induced reactions.
- CO-4 Students will be able to understand the electron transfer reactions in metal complexes.
- CO-5 Students will be able to understand bridged outer-sphere electron transfer mechanism, Nucleophilic and electrophilic catalyst and their mode of action.

Unit I

Micelles catalysis and inhibition

Kinetics and mechanism of micelle catalyzed reactions (1st order and second order) Various type of micelle catalyzed reactions. Micelle inhibited reactions.

Kinetics and Mechanism of Substitution Reaction

Classification of ligand substitution mechanism. Anation and base catalyzed kinetics of anation reactions. Aquation and acid catalyzed kinetics of aquation reactions (octahedral complexes).

Unit II

Radiation Chemistry

Radiation chemistry and photochemistry. Radiation chemistry of water and aqueous solutions. Hydrogen atom and hydroxyl radical-oxidizing and reducing conditions. Kinetics and

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mechanism of photochemical and photosensitized reactions (One example in each case). Stern-Volmer equation and its application. Hole-concept in the presence of semiconductor type photocatalysts. Kinetics and mechanism of electron transfer reaction in the presence of visible light. Kinetics of exchange reactions (Mathematical analysis)

Unit III

Induced Phenomenon

Induced reactions concept and their characteristics, Induction factor, Mechanism of (i) Fe (II) induced oxidation of iodine by Cr(VI) in weak acid medium, (ii) As (III) induced oxidation of Mn(II) by chromate in acid solutions. Kinetics and mechanism of induced reactions in metal complexes (octahedral complexes of Cobalt (III) only)-basic concepts.

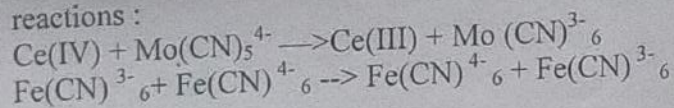
Unit IV

Electron Transfer Reaction in Metal Complexes

Kinetics and mechanism of 1:1, 1:2, 1:3 metal substrate complexes as intermediate, Henry Taubes classical reaction, its kinetics and mechanism, Inner-sphere and outer sphere, electron transfer reactions and mechanism. Various types of inner sphere bridges, adjacent and remote attack. Linkage isomerism. Chemical and resonance mechanism.

Unit V

Marcus-Cross relation in outersphere reactions (no mathematical derivation). Its application in reactions :



Bridged outer-sphere electron transfer mechanism, Nucleophilic and electrophilic catalyst and their mode of action.

Suggested Books References:

1. Progress in Inorganic Chemistry, Vol. 30 1967.
2. R. Lumry and R.W. Raymond, Electron Transfer Reactions, Interscience.
3. N.L. Bender, Mechanism of Homogeneous Catalysis from protein to protein, Wiley.
4. A.G. Sykes, Kinetics of Inorganic reactions, Pergamon.
5. S.W. Benson, Mechanism of Inorganic Reactions, Academic Press.
6. Physical Chemistry Vol. 2, Ed. Prof Ya Grasimov, Mir publisher.
7. Basolo and Pearson, Inorganic Reaction Mechanisms, Wiley.
8. H. Taube, Electron Transfer Reactions, Oxford Press

MCE 038A : Polarography and Chemical Kinetics (Practical)

1. Identification and estimation of metal ions such as Cd^{+2} , Pb^{+2} , Zn^{+2} , polarographically.
2. Study of a metal ligand complex polarographically (using Lingane's Method).

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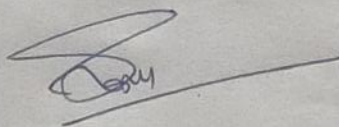
3. Determination of rate constant and formation constant of an intermediate complex in the reaction of Ce(IV) and Hypophosphorous acid at ambient temperature.
4. Determination of energy and enthalpy of activation in the reaction of KMnO_4 and benzyl alcohol in acid medium.
5. Determination of energy of activation of and entropy of activation from a single kinetic run.
6. Kinetics of an enzyme catalyzed reaction
7. To determine the hardness of Water by complexometric method and by HCl method.
8. To determine the amount of free chlorine in given water sample.
9. Determination of Total residual Chlorine and amount of Fluoride ion in given water samples.
10. Determination of Viscosity of a given lubricant by Redwood Viscometer No.1.
11. Determination of Flash and Fire Points of a given lubricant by Pensky Martin Apparatus.
12. Determination of Cloud and Pour Points of a given lubricant.
13. To determine moisture, volatile and ash content in a given coal sample by proximate analysis.
14. To determine the calorific value of Solid Fuel by Bomb's Calorimeter.

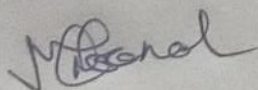
Books Suggested

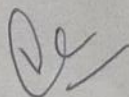
1. Inorganic Experiments, J. Derek Woolings, VCH.
2. Microscale Inorganic Chemistry, Z. Szafran, R.M. Pike and M.M. Singh, Wiley.
3. Practical Inorganic Chemistry, G. Marr and B. W. Rockett, Van Nostrand.
4. The systematic Identification of Organic Compounds, R.L. Shriner and D.Y. Curtin.

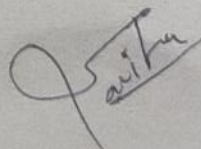
MCE 041A : Minor Project : (Which will be done in vacations after Semester-III and will be evaluated in Semester-IV)

28

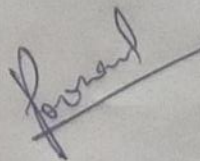








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