SYLLABUS

M.Sc. in Chemistry

REGULAR COURSE

UNDER CBCS SYSTEM

(FROM SESSION- 2023-24 & ONWARDS)

AFFILIATED TO

UTKAL UNIVERSITY

VANI VIHAR, BHUBANESWAR

P.G. DEPARTMENT OF CHEMISTRY

GOVINDPUR (DEGREE) COLLEGE

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UTKAL UNIVERSITY
COURSE OF STUDIES
FOR THE
M. Sc. EXAMINATION IN CHEMISTRY

(2020-2021)

PREFACE

Master of Science (M.Sc.) in Chemistry is a full time two years post-graduation programme of Utkal University. The choice based credit system (CBCS) syllabus in M. Sc. Chemistry is comprised of four semesters, having total of 94 credits (1800 marks). There are 20 theory papers carrying three credits each with 70 full marks. Out of which mid and end semester examinations carry 20 marks and 50 marks, respectively. The duration of end semester examination is two hours. Besides there are 7 practical papers (4 credit each and full mark 50) with end semester examination of six hours duration. The fourth semester has a compulsory project work of 6 credit (50 marks). Students are required undertake a project work after completion of 2^{nd} semester and submit project report in the 4^{th} semester for evaluation.

Questions will be set unit wise with long and short answer type questions. Each unit will carry 2 questions. Students are required to answer 3 questions with one question from each unit. The question paper will comprise both subjective and objective with problem oriented approach.

PROGRAM OBJECTIVES:

- To impart knowledge in fundamental aspects of all branches of chemistry (Organic, Inorganic, Physical and Polymer Chemistry) along with the current scientific status and new developments in Chemistry.
- To acquire deep knowledge in the specific areas like spectroscopy, solid state chemistry, environmental chemistry etc.
- To teach the students about good laboratory practices, safety of oneself and others in the laboratory.
- To acquire the different practical skills, hand on training on basic equipment, and data analysis for research and better job prospective.
- To train the students in accepting the challenges in Chemistry and to become a responsible citizen in the society.

PROGRAM OUTCOMES:

On completion of the M.Sc. Chemistry programme, the students will:

- Acquire the in-depth functional knowledge of the fundamental principles and contemporary practices of chemistry and ability to use them to investigate, explain and predict the new phenomena.
- Acquire skills to design, execute and document of laboratory experiments at a level suitable to succeed at an entry level position in research, academia, or chemical industry.
- Develop an awareness of social, economic, environmental and technological implication of chemistry.
- Find job opportunities in Chemical, pharmaceutical, and other chemistry based industries; Research & Development in various scientific/academic institutions.
- Have the ability to disseminate research results orally, and in writing.

Structure of syllabus for Semester Pattern Choice based credit system M.Sc. (Chemistry) Programme effective from the session- 2020 - 2021

SEMESTER I

Core Paper	**Subject (Paper)**	**Code**	**Credit**	**Full Marks**	**Total Marks**
Theory	Inorganic Chemistry-I	CH-401	3	70	**450**
Theory	Organic Chemistry- I	CH -402	3	70	
Theory	Physical Chemistry –I	CH -403	3	70	
Practical	Inorganic Chem. Practical-I	CH -404	4	50	
Practical	Organic Chem. Practical-I	CH -405	4	50	
Allied Elective					
Theory	Spectroscopy-I	CH -406	3	70	
Theory	Computer for Chemist	CH -407	3	70	

SEMESTER II

Core Paper	**Subject (Paper)**	**Code**	**Credit**	**Full Marks**	**Total Marks**
Theory	Inorganic Chemistry-II	CH -408	3	70	**450**
Theory	Organic Chemistry-II	CH -409	3	70	
Theory	Physical Chemistry-II	CH -410	3	70	
Practical	Inorganic Chem. Practical-II	CH -411	4	50	
Practical	Organic Chem. Practical-II	CH -412	4	50	
Allied Elective					
Theory	Spectroscopy-II	CH -413	3	70	
Theory	Analytical Chemistry	CH-414	3	70	

SEMESTER III

Core Paper	**Subject (Paper)**	**Code**	**Credit**	**Full Marks**	**Total Marks**
Theory	Pericyclic reactions and photochemistry	CH -501	3	70	**450 (Marks of Add on course is not included)**
Theory	Bioinorganic & Supramolecular Chemistry	CH -502	3	70	
Practical	Applied Chemistry Practical	CH -503	4	50	
Practical	Physical Chemistry Practical-I	CH -504	4	50	
Allied elective					
Theory	Application of Spectroscopy-I	CH -505	3	70	
Theory	Organic Synthesis	CH -506	3	70	
Allied elective for M.Sc. Students and Free elective for other discipline					
Theory	Environmental Chemistry	CH -507	3	70	
****Add on Course***					
Theory	Techniques of Chemical Analysis	CH-ADD1	4	50	

SEMESTER IV

Core Elective Papers	**Subject (Paper)**	**Code**	**Credit**	**Full Marks**	**Total Marks**
Theory	Bioorganic Chemistry	CH -508	3	70	**450**
Theory	Organotransition metal chemistry	CH -509	3	70	
Theory	Polymer Chemistry	CH -510	3	70	
Theory	Solid State Chemistry	CH -511	3	70	
Practical	Physical Practical -II	CH -512	4	50	
Project	Project work and Seminar	CH -513	6	50	
Allied Elective					
Theory	Application of Spectroscopy-II	CH -514	3	70	
Total Credit = 94, Total full marks = 1800					

***Allied departments are Physics, Zoology, Botany, Biotechnology, Geology, and Computer Science**
*** Free elective is open for students from any discipline.**
*****Add on course is open to M. Sc. students of Physics, Chemistry, Zoology, Botany, Biotechnology, Geology and Pharmacy. ***Add on course is open to any discipline of Utkal University**

SEMESTER-I

(Two questions to be set from each Unit. Students are required to answer one question from each unit)

CH 401: INORGANIC CHEMISTRY-I

Mid Sem: 20 marks
End Sem: 50 marks

Objective:

(i) To understand the concepts of bonding and stereochemistry of main group elements, (ii) To learn about the formation and stability of metal complexes and their determination and (iii) Mechanistic aspects of different types of reaction of metal complexes in solution.

Outcome: At the end of the course the student will

(i) Acquire the knowledge and have the ability to describe the bonding and stereochemistry of different inorganic compounds and ions. (ii) Be able understand the concept stability constant, its determination and application in different fields (iii) Understand the reactions and mechanism of different types of reactions in coordination compounds and their applications in practical fields.

UNIT I

Stereochemistry and Bonding in Main Group Compounds

VSEPR, Bent rule and energetics of hybridization, Walsh diagrams (tri-and penta-atomic molecules), d_π-p_π bonds, some simple reactions of covalently bonded molecules.

Wade's rule, Styx number, carboranes, isolobal analogy, Lipscom topology, applications of boron compounds, synthesis and structures of S-N cyclic compounds.

UNIT II

Metal –Ligand Equilibria in Solution

Stepwise and overall formation constants and their interaction, trends in stepwise constants, factors affecting the stability of metal complexes with reference to the nature of metal ions and ligands, chelate and macrocyclic effect and their thermodynamic origin, determination of binary formation constants by pH- metry and spectrophotometry.

UNIT III

Reaction Mechanism of Transition Metal Complexes

Energy profile of a reaction, reactivity of metal complexes, inert and labile complexes, kinetic applications of valence bond and crystal field theories, 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 one electron transfer reactions, outer sphere type reactions, cross reactions and Marcus-Hush theory, Inner sphere type reactions

Books Recommended:

1. Advanced Inorganic Chemistry, F. A. Cotton, M. Bochmann, C. A. Murillo, G. Wilkinson, 6th Ed., Wiley India (2007).
2. Inorganic Chemistry, J. E. Huheey, E. A. Keiter, R. L. Keiter, O. K. Medhi, 4th Ed., Pearson Education (2006).
3. Chemistry of the Elements, N.N. B. Greenwood and A. Earnshow, Pergamon, 2nd Ed (1997)
4. Inorganic Electronic Spectroscopy, A. B. P. Lever, Elsevier, 2nd Ed., (1984).
5. Comprehensive Coordination Chemistry eds., G. Wilkinson, R. D. Gillards and J. A. McCleverty, Pergamon (2003).
6. Fundamental Concepts of Inorganic Chemistry, Vol. 2, 4 & 5; Asim K. Das, CBS Publisher, 2nd Ed., (2013).
7. Mechanism of Inorganic Reactions, F. Basolo and R.G. Pearson, Wiley Eastern, (1967).

8. Inorganic Chemistry, K.F. Purcell & J.C. Kotz, Cengage Learning, Indian Ed., (2010).
9. Concepts and Models of Inorganic Chemistry, B. Douglas, D. McDaniel, J. Alexander, Willey, 3rd Ed., (2006).

CH 402: ORGANIC CHEMISTRY-I

Mid Sem: 20 marks
End Sem: 50 marks

Objective:

To understand the molecular details in greater depth on following topics: aromaticity, stereochemistry, and substitution reactions in aliphatic compounds.

Outcome:

Upon completion of this course students will be able to: (i) Understand the fundamental aspects of aromaticity, nonaromaticity and antiaromaticity, (ii) Feel the structural details of organic compounds and the origin of optical activity of the chiral molecules, (iii) Understand the origin of stereoselectivity as far as asymmetric catalysis is concern, and the basic mechanism of substitution reactions in aliphatic compounds.

UNIT I

Structure, Reactivity and Bonding in Organic Molecules

Delocalized chemical bonding-conjugation, cross conjugation, resonance, hyperconjugation, bonding in fullerenes, tautomerism. Aromaticity in benzenoid and non-benzenoid compounds, alternant and non-alternant hydrocarbons, Huckel's rule, energy level of π- molecular orbitals, annulenes, antiaromaticity, ψ-aromaticity, homo-aromaticity, PMO approach. Bonds weaker than covalent addition compounds, crown ether complexes and cryptands, inclusion compounds, cyclodextrins, Catenanes and Rotaxanes.

Types of mechanisms, types of reactions, thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammond's postulate, Curtin-Hammett principle. Potential energy diagrams, transition states and intermediates, methods of determining mechanisms, isotope effects. Hard and soft acids and bases.

Effect of structure on reactivity- resonance and field effects, steric effect, quantitative treatment. The Hammett equation and linear free energy relationships, substitutent and reaction constants. Taft equation.

UNIT II

Stereochemistry

Conformational analysis of cycloalkanes, decalins, effect of conformation on reactivity, conformation of sugars, steric strain due to unavoidable crowding.

Elements of symmetry, chirality, molecules with more than one chiral center, threo and erythro isomers, methods of resolution, optical purity, enantiotropic and diastereotropic atoms, groups and faces, stereospecific and stereoselective synthesis. Asymmetric synthesis using chiral reagent, chiral catalysts, chiral auxiliary and chiral substrates (*Felkin-Anh* model and *Cram's* rule). Optical activity in the absence of chiral carbon (biphenyls, allenes, spiranes, transcycloalkene and metallocenes), chirality due to helical shape.

UNIT III

Aliphatic Nucleophilic Substitution

The S_N2, S_N1, S_Ni mixed S_N1 and S_N2 and SET mechanisms. The neighbouring group mechanism, neighbouring group participation by π and σ bonds, anchimeric assistance

Nucleophilic substitution at an allylic, aliphatic trigonal and a vinylic carbon.

Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium, phase transfer catalysis and ultrasound, ambident nucleophile, regioselectivity.

Aliphatic Electrophilic Substitution

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

Books Recommended

1. Advanced Organic Chemistry-Reactions, Mechanism and Structure, Jerry March, John Wiley.
2. Advanced Organic Chemistry, F.A. Carey and R. J. Sundberg, Plenum.
3. A Guide Book of Mechanism in Organic Chemistry, Peter Sykes, Longman.
4. Structure and Mechanism in Organic Chemistry, C. K. Ingold, Cornell University Press.
5. Organic Chemistry, R. T. Morrison and R. N. Boyd, Prentice-Hall.
6. Modern Organic Reactions, H. O. House, Benjamin.
7. Principles of Organic Synthesis, R.O.C. Norman and J.M.Coxon, Blackie Academic & Professional.
8. Pericyclic Reactions, S. M. Mukherji, Macmillan, India.
9. Reaction Mechanism in Organic Chemistry, S.M. Mukherjee and S.P. Singh, Macmillan.
10. Stereochemistry of Organic Compounds, Ernest L. Eliel and Samuel H. Wilen, Wiley.
11. Stereochemistry of Organic Compounds, D. Nasipuri, New Age International.
12. Basic Stereochemistry of Organic molecules, Subrata Sen Gupta, Oxford University Press; First edition.
13. Organic synthesis: Clayden, Greeves, Warren and Wouthers, Oxford Univ. Press.

CH 403: PHYSICAL CHEMISTRY-I

Mid Sem: 20 marks
End Sem: 50 marks

Objective:

The topics covered under the course are inherently very fundamental and intended to provide the basic understanding at atomic and subatomic level. The objective of the course to study and understand the concept of energy, the transfer of energy into work, capacity of energy to function, entropy, enthalpy, chemical potentials, thermodynamic laws, criterion for determination of the feasibility or spontaneity of a given transformation, partial molar properties, their determinations. The course is designed in a manner in which a bridge between classical thermodynamics and quantum mechanics can be established.

Outcome:

Understanding the underlying concepts and realization of quantum mechanics will be useful in solving problems at realistic atomic and molecular level, in particularly in the field of spectroscopy and analytical chemistry. Understanding thermodynamics requires knowledge of how the microscopic world operates and importance of reversible and irreversible processes.

UNIT I

Quantum Chemistry

Introduction to Exact quantum Mechanical Results

Postulates of quantum mechanics, Schrodinger equation and discussion of solutions of the Schrodinger equation to some model systems viz., particle in a box, the harmonic oscillator, the rigid rotator, the hydrogen atom.

Approximate Methods

The variation theorem, linear variation principle. Perturbation theory (first order and non-degenerate). Applications of variation method and perturbation theory to the Helium atom.

Angular Momentum

Ordinary angular momentum, generalized angular momentum, eigenfunctions for angular momentum, eigenvalues of angular momentum, operator using ladder operators, addition of angular moments, spin, antisymmetry and Pauli exclusion principle.

Molecular Orbital Theory

Huckel theory of conjugated systems, bond order and charge density calculations. Applications to ethylene, butadiene, cyclopropenyl radical, cyclobutadiene etc.

UNIT II

Thermodynamics

Classical Thermodynamics

Concept of free energy, chemical potential and entropy. Partial molar properties; partial molar free energy, partial molar volume and partial molar heat content and their significances and determinations. Concept of fugacity and determination of fugacity.

Non-ideal systems: Excess functions for non-ideal solutions. Activity, activity coefficient.

Non Equilibrium Thermodynamics

Thermodynamic criteria for non-equilibrium states, entropy production and entropy flow, entropy balance equations for different irreversible processes (e.g., heat flow, chemical reaction etc.) transformations of the generalized fluxes and forces, non equilibrim stationary states, phenomenological equations

UNIT III

Statistical Thermodynamics

Thermodynamic probability concept of ensemble. Ensemble averaging, postulates of ensemble averaging. Canonical, grand canonical and microcanonical ensembles, corresponding distribution laws (using Lagrange's method of undetermined multipliers) Maxwell- Boltzmann, Bose-Einstein and Fermi Dirac statistics.

Partition functions-translational, rotational, vibrational and electronic partition functions, calculation of thermodynamic properties in terms of partition functions. Applications of partition functions.

Heat capacity behaviour of solids-chemical equilibria and equilibrium constant in terms of partition functions, Fermi–Dirac statistics, applications to metal. Bose-Einstein statistics-application to helium. Bose-Einstein condensate.

Books Recommended

1. Physical Chemistry , P.W.Atkins and J. D. Paulo, Oxford, 2013, 10th edition New Delhi.
2. Introduction to Quantum Chemistry, A.K.Chandra, Tata McGraw Hill, 1997, 4th edition, New Delhi.
3. Quantum Chemistry, Ira N. Levine, Pearson, 2007, 5th edition, New Delhi.,
4. Quantum Chemistry, D. A. McQuarrie and Simon, Viva, 2007, 1st edition, New Delhi.
5. Molecular Quantum Mechanics, Atkins and Friedman, Oxford Univ. Press, 1997, 3rd edition, New York.
6. Quantum Chemistry, J. P. Lowe, Academic Press, 2nd edition, New York.
7. Quantum Chemsitry- R.K. Prasad, New Age International (P) Ltd
8. Quantum Chemsitry through problems and solution- R. K. Prasad, New Age International (P) Ltd
9. A textbook of Physical chemistry – H.K. Moudgil
10. Physical Chemistry, T. Engel and P. Reid, Pearson, 2006, 1st edition, New Delhi.
11. Thermodynamics, G. N. Lewis and M. Randall, McGraw Hill, 2nd edition, 1961, New York.
12. Molecular Thermodynamics, D. A. McQuarrie and Simon. Viva, 2009, 1st edition, New Delhi.
13. Non Equilibrium Thermodynamics, S.R. deGroot and Mazur, Dover, New York.
14. Introductory Statistical Thermodynamics, T. Hill, Dover, 1986, New York.
15. Statistical Thermodynamics, Oxford, Oxford Chemistry Primer vol. 58, 1997.
16. Introduction to Statistical Mechanics, R. Bowley and M. Sanchez, Clarendon press,
17. Statistical Mechanics and Thermodynamics, C. Garrod, Oxford Univ. Press, 1995, New York.
18. Introduction to thermodynamics of irreversible processes, 2nd edition, Interscience, 1961, New York.

CH 404: INORGANIC CHEMISTRY PRACTICAL-I

Full Marks 50

Objective:

(i) Qualitative analysis of inorganic salts mixture containing acid and basic radicals with insoluble compound (ii) To separate the mixture of cations and anions by chromatographic technique (iii) To learn the best laboratory practice

Outcome:

(i) Ability to separate and identify different cations and anion from a mixture of inorganic salts. (ii) Understanding the principles of separation and analysis of different ions and their applications in real fields. (iii) Learn the techniques of chromatographic separation of mixture of cations and anions

Qualitative Analysis of inorganic mixture

Semi micro qualitative analysis of inorganic mixtures containing anions, common cations, less common metal ions (W, Mo, Ce, Th, Zr, V and U) and insoluble (sulphate, oxides, halide).

Ion Exchange Chromatography

Separation of mixture of cations and anions by

(a) Paper Chromatography

(b) Column Chromatography – Ion exchange: Co(II)/Ni(II); Cd(II)/Mg(II)

Books recommended

1. Inorganic Experiments, J. Derck Woollins., 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. An Advanced Course of Practical Chemistry, Nad, Ghosal & Mahapatra, Central Publisher (2000).
5. Vogel's Qualitative Inorganic Analysis, 7^{th} Ed, Revised by G. Svehela, 4^{th} Ed., Person (2007).

CH 405: ORGANIC CHEMISTRY PRACTICAL-I

Full Marks-50

Objective:

To introduce the theory and procedures of qualitative analysis of unknown organic compounds in a mixture by conventional methods as well by chromatography and IR spectra.

Outcome:

Upon completion of this course students will be able to

1) Understand how to detect the presence of different functional groups
2) Demonstrate/apply the techniques involved in organic binary mixture separation
3) Understand how to characterize different functional groups using IR spectroscopy technique.
4) Understand the art of identifying the unknown organic compounds.

Qualitative Analysis

Identification of unknown organic compounds, separation, purification and identification of compounds of binary mixture (both are solids, one liquid & one solid) using TLC & column chromatography, Chemical tests. IR spectra to be used for functional group identification.

Books Recommended

1. Experiments and Techniques in Organic Chemistry, D.Pasto, C.Johnson, & M. Miller, Prantice Hall.
2. Systematic Qualitative Organic Analysis, H. Middleton, Edward Arnold (Publisher).
3. Hand Book of Organic Analysis, Qualitative & Quantitative, M.T.Clarke, Edward Arnold (Publisher).
4. Vogel's Text Book of Practical Organic Chemistry, A.R. Tatchell, John Wiley.
5. Macroscale and Microscale Organic Experiments, K.L.Williamson, D.C.Heath.
6. A Text Book of Practical Organic Chemistry (Qualitative). Arthur I.Vogel.

CH 406: SPECTROSCOPY- I

Unit Pattern

Mid Sem: 20 marks
End Sem: 50 marks

Objective:

(i) To introduce the concept of symmetry and group theory and their application in chemistry (ii) to provide theoretical basis of understanding the atomic, molecular, microwave and photoelectron spectroscopies and their applications.

Outcome:

Completion of the course will enable the students (i) to understand importance group symmetry and group theory in chemistry, classifying different compounds in to point groups and derive the character tables for various applications. (ii) to explain the theory and applications atomic, molecular and microwave spectroscopy (iii) to explain the basic principles of photoelectron spectroscopy and its application to chemical analysis.

UNIT I

Symmetry and Group Theory in Chemistry

Symmetry elements and symmetry operation, definitions of group, subgroup, relation between orders of a finite group and its subgroup. Conjugacy relation and classes. Generators, Point symmetry group.

Representations of group operators, The great orthogonality theorem (without proof) and its explanation. Irreducible and reducible representation. Bases of representation, Character of a representation. Character table and its meaning. Reduction formula.

Unifying Principles

Interaction of electromagnetic radiation with matter: absorption, emission, transmission, Uncertainty relation and natural line width and natural line broadening, transition probability, results of the time dependent perturbation theory, transition moment, and intensity of spectral lines.

UNIT II

Atomic Spectroscopy

Energies of atomic orbitals, vector representation of momenta and vector coupling, Electronic configuration, Russell-Saunders terms and coupling schemes, magnetic effects: spin-orbit coupling and Zeeman splitting, spectra of hydrogen atom and alkali metal atoms.

Molecular Spectroscopy

Energy levels, molecular orbitals, vibronic transitions, vibrational progressions , Franck-Condon principle, Electronic spectra of diatomic molecules, electronic spectra of polyatomic molecules. Emission spectra; radiative and non-radiative decay, internal conversion,

Spectra of transition metal complexes (d^1 and d^9 system), charge-transfer spectra

UNIT III

Photoelectron Spectroscopy

Basic principles; photo-electric effect, ionization process, Koopman's theorem. Photoelectron spectra of simple molecules (H_2, O_2, N_2, CO, H_2O), Spectroscopy of core electrons-Electron Spectroscopy of Chemical Analysis, Chemical information from ESCA. Auger electron spectroscopy – basic idea.

Microwave Spectroscopy

Classification of molecules, rigid rotor model, effect of isotopic substitution on the transition frequencies, intensities, non-rigid rotor, Stark effect, nuclear and electron spin interaction and effect of external field, Applications.

Books Recommended

1. Modern Spectroscopy, J.M. Hollas, John Wiley, 4th edition, Sussex.
2. Applied Electron Spectroscopy for Chemical Analysis Ed. H. Windawi and F.L.Ho, Wiley Inter science.
3. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, R.V. Parish, Ellis Harwood, 1st edition, 1990.
4. Physical Methods in Chemistry, R.S.Drago, Sauders College (1992).
5. Chemical Applications of Group Theory, F.A. Cotton. Wiley Inter science, 3rd ed., (1990).
6. Symmetry and Spectroscopy of Molecules, , K.V. Reddy, New Age International (P) Ltd., Ist Ed., (1998).
7. Introduction to Molecular Spectroscopy, G.M.Barrow, McGraw Hill
8. Basic Principles of Spectroscopy, R.Chang, McGraw Hill.
9. Theory and Applications of UV Spectroscopy, H.H.Jaffe and M.Orchin, IBH-Oxford.
10. Introduction to Photoelectron Spectroscopy, P.K.Ghosh, John Wiley.
11. Introduction to Magnetic Resonance, A. Carrington and A.D. Maclachalan, Harper & Row.
12. Inorganic spectroscopic methods, A.K. Brisdon, Oxford Chem. Primers, 1997, New York.
13. Spectroscopy, S. Walker and H. Straw, Chapman and Hall ltd.
14. Energy levels in atom and molecules, W.G. Richards and P.R. Scott, Oxford, Oxford Chemistry Primer vol. 26, 1994, New York.
15. Atomic Spectra, T.P. Softley, Oxford, Oxford Chemistry Primer, Vol. 19, New York.
16. Introduction to Spectroscopy, Pavia, Brooks/Cole Cenage, 4th edition, 2009, Belmont.
17. Electronic Absorption Spectrocopy and related Techniques- D. Sathyanarayanan
18. Fundamental concept of Inorganic Chemistry vol-7- A.K. Das and Mahua Das, CBS Publisher
19. Fundamental of Molecular Spectroscopy- C. N Banwell, Tata McGraw Hill

CH 407: COMPUTERS FOR CHEMISTS

Unit pattern

Mid Sem: 20 marks
End Sem: 50 marks

Objective:

This is a theory-cum-Laboratory course with more emphasis on laboratory work. The objectives are to study different computer programmes, to learn various concepts and basic techniques essential for conduct of practical in computers and to study various computer languages useful in Chemistry.

Outcome:

After the completion of course students will able to acquire basic understanding about Computer, computer programmes, computer languages, understanding the basic concept associated with C- and C^{++} Language and program designing, develop different programs,

Run and Retrieve results, use of variables, arithmetic assignment operators and conditional operator, and in future student may be able to develop a big program(s)(Software) which may simulate the behaviour of the chemical reaction/processes/events.

UNIT I

Computer Programming in C

Elements of the computer language, Constants and variables, Operations and symbols. Expressions, Arithmetic assignment statement. Input and Output, Format statement. Termination statements, Branching statements such as IF, ELSE-IF Statements; Nested loop, Loop control statement. FUNCTION (Students learn the programming logic and these language features by 'hands on' experience on a personal computer from the very beginning of this topic).

UNIT II

Programming in Chemistry

Development of small computer codes involving simple formulae in chemistry, such as vander Waals equation, pH titration, kinetics, radioactive decay. Evaluation of lattice energy and ionic radii from experimental data. Linear simultaneous equations to solve secular equations within the Huckel theory. Elementary structural features such as bond lengths, bond angles, dihedral angles etc. of molecules extracted from a database such as cambridge data base.

UNIT III

Use of Computer Programmes

The students will learn how to operate a PC and how to run standard programmes and packages. Execution of linear regression, X-Y plot, numerical integration and differentation as well as differential equation solution programmes.

Use of Computer Programmes

Programmes with data preferably from Physical Chemistry Laboratory. Further, the students will operate the packages MS- WORD, POWER POINT AND EXCEL.

Books Recommended

1. Computers and Common Sense, R. Hunt and J. Shelley, Prentice Hall
2. Computational Chemistry, A.C. Norris.
3. Microcomputer Quantum Mechanics, J.P. Killngbeck, Adam Hilger.
4. An Introduction to Digital Computer Design, V.Rajaraman and T. Radhakrishnan, Prentice Hall.
5. Computer and their applications to Chemistry, R. Kumari, 2nd Edn,Narosa (2005).

SEMESTER-II

CH 408: INORGANIC CHEMISTRY-II

Mid Sem: 20 marks
End Sem: 50 marks

Objective:

1. To understand the theoretical basis of boding of structurally different coordination compounds.
2. To understand the basis of electronic spectra of metal complexes as well as to understand the basis of anomalous magnetic behaviour of metal complexes.
3. To impart knowledge on preparative methods, structure and bonding of metal-π complexes and cultures.

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

1. Understand and explain the bonding in coordination and organometallic compounds. Describe the fundamental requirement to interpret the electronic spectra of metal complexes for prediction of their properties.
2. Describe the synthesis, structure and bonding of metal carbonyls, metal nitrosyls, dioxygen, dinitrogen complexes as well as metal clusters.

UNIT I

Metal-Ligand Bonding

Crystal Field Theory and its limitations, Elementary idea of Angular overlap model, Molecular orbital theory for octahedral, tetrahedral and square planar complexes, σ and π-bonding in molecular orbital theory.

UNIT II

Electronic Spectra and Magnetic Properties of Transition Metal Complexes.

Spectroscopic ground states, correlation, Orgel and Tanabe-Sugano diagrams for transition metal complexes (d^1 –d^9 states), calculations of Dq, B and β parameters, charge transfer spectra, spectroscopic method of assignment of absolute configuration in optically active metal chelates and their stereo-chemical information, anomalous magnetic moments, magnetic exchanges coupling and spin crossover.

UNIT III

Metal π-Complexes

Metal Carbonyls, Structure and bonding, Vibrational spectra of metal carbonyls for bonding and structural elucidation, important reactions of metal carbonyls. Preparation, bonding, structure and important reactions of transition metal nitrosyls, dinitrogen and dioxygen complexes, ligating behavior of tertiary phosphines.

Metal Clusters

Higher boranes, carboranes, metalloboranes and metallocarboranes. Metal carbonyl and halide clusters, compounds with metal-metal multiple bonds.

Books Recommended:

1. Advanced Inorganic Chemistry, F. A. Cotton, M. Bochmann, C. A. Murillo, G. Wilkinson, 6th Ed., Wiley India (2007).
2. Inorganic Chemistry, J. E. Huheey, E. A. Keiter, R. L. Keiter, O. K. Medhi, 4th Ed., Pearson Education (2006).
3. Chemistry of the Elements, N.N. B. Greenwood and A. Earnshow, Pergamon, 2nd Ed (1997)
4. Inorganic Electronic Spectroscopy, A.B.P.Lever, Elsevier.
5. Magnetochemistry, R.L.Carlin, Springer Verlag.

6. Comprehensive Coordination Chemistry eds., G.Wilkison, R.D.Gillars and J.A.McCleverty, Pergamon.
7. Elements of Magneto Chemistry, R. L. Dutta, A. Syamal; 2nd Ed. East West Press Pvt Ltd (2009).
8. Fundamental Concepts of Inorganic Chemistry, Vol. 5; Asim K. Das, CBS Publisher, (2015).
9. Fundamental Concepts of Inorganic Chemistry, Vol. 6; Asim K. Das, CBS Publisher, 2nd Ed., (2013).
10. Organometallic Chemistry, R.C. Mehrotra & A. Singh, New Age International, 2nd Ed (2013).
11. Inorganic Chemistry, C. L. Miessler, D. A. Tarr, Pearson, 3rd Ed., (2004).

CH 409: ORGANIC CHEMISTRY-II

Unit pattern

Mid Sem: 20 marks
End Sem: 50 marks

Objective:
To impart knowledge of substitution reactions of aromatic compounds, addition reactions to carbon-carbon and carbon-heteroatom multiple bonds, and rearrangement of reactive intermediates.

Outcome: Upon completion of this course students will be able to understand the basic principle of substitution reaction in aromatic compounds along with reaction mechanism, Understand the mechanism of addition reactions of carbon-carbon (C=C C≡C, etc.) multiple bonds and carbon-heteroatom (C=O, C=N, etc.) multiple bonds, and the structure and reactivity of various reactive intermediates.

UNIT I

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, Vilsmer reaction, Gattermann-Koch reaction.

Aromatic Nucleohilic Substitution

The S_NA_r, S_N1, Benzyne and $S_{RN}1$ mechanisms. Reactivity- effect of substrate structure, leaving group and attacking nucleophile. The von Richter, Sommelet-hauser, and Smiles rearrangements.

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 halogenatin (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

Addition to Carbon-Carbon Multiple Bonds

Mechanistic and stereochemical aspects of addition reactions Hydrogenation, Halogenation, Hydrohalogenation, Hydroboration, Oxymercuration, Sulfenylation, Seleneylation, 1, 3-dipolar species addition, Hydoxylation: Prevost & Woodward hydroxylation, Using $KMnO_4$

and OsO_4, Epoxidation, Sharpless asymmetric epoxidation, Michael reaction, Prins reaction, Addition to cyclopropane ring, Addition to conjugated system.

Addition to Carbon-Hetero Multiple Bonds

Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acids, esters and nitriles. Addition of Grignard reagents, organozinic and organolithium regents to carbonyl and unsaturated carbonyl compounds. Witting reaction.

Mechanism of condensation reactions involving enolates – Aldol, Konevenagel, Claisen, Mannich, Benzoin, Perkin and Stobbe reactions.

UNIT III

Rearrangements

Generation, structure, stability and reactivity of Classical and nonclassical carbocations, phenonium ions, norbornyl system, carbanions, free radicals, benzyne, carbenes and nitrenes.

General mechanistic considerations – nature of migration, migratory aptitude, memory effects. A detailed study of the following rearrangements

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

Elimination Reactions

The E_2, E_1 and E_1cB mechanisms and their spectrum. Orientation of the double bond. Reactivity – effects of substrate structures, attacking base, the leaving group and the medium. Mechanism and orientation in pyrolytic elimination.

Books Recommended

1. Advanced Organic Chemistry-Reactions, Mechanism and Structure, Jerry March, John Wiley, 6th Ed., (2006).
2. Advanced Organic Chemistry, F. A. Carey and R. J. Sundberg, Part A and B Springer, 5th Ed., (2005).
3. A Guide Book of Mechanism in Organic Chemistry, Peter Sykes, Longman.6th Ed., (1999).
4. Structure and Mechanism in Organic Chemistry, C. K. Ingold, Cornell University Press, 3rd Ed., (1957).
5. Organic Chemistry, R. T. Morrison and R. N. Boyd, Prentice-Hall.
6. Modern Organic Reactions, H. O. House, W.A. Benjamin. 2nd Ed., (1972).
7. Principles of Organic Synthesis, R.O.C. Norman and J. M. Cox, CRC Press 3rd Ed., (2014).
8. Reaction Mechanism in Organic Chemistry, S. M. Mukherjee and S. P. Singh, Macmillan.3rd Ed., (2009).

CH 410: PHYSICAL CHEMISTRY-II

Mid Sem: 20 marks
End Sem: 50 marks

Objective: Chemical kinetics is the study of the rates of chemical reactions, factors which are influential in the rates and the explanation of the rates with respect to the reaction mechanisms of chemical processes. The course content is designed to provide a fundamental understanding

of basic surface properties such as surface tension, capillarity and adsorption etc. Also the content describes the importance and application of surfactants, starting from basic definition to micelle formation and factors responsible for micelle formation. This course contents have a balance between conventional and modern electrochemistry.

Outcome: Students can follow the concept of rate of change associated with chemical reaction, recognizing that the rate of change and how it can be measured. Learning and discussion of surface chemistry certainly enable a student to solve problems associated with catalysis and nanochemistry, as most of the reactions are observed at the interface. It is believed that after going through the course a student will find its utility in chemistry of batteries, fuel cells, solar cells etc.

UNIT I

Chemical Dynamics

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

Dynamic chain (hydrogen-bromine reaction, pyrolysis of acetaldehyde, decomposition of ethane), photochemical (hydrogen- bromine and hydrogen-chlorine reactions) and oscillatory reations (Belousov-Zhabotinsky reaction), homogeneous catalysis, kinetics of enzyme reactions, general features of fast reactions, study of fast reactions by stopped flow method, relaxation method, flash photolysis, Diffusion controlled reaction, dynamics of molecular motion.

UNIT II

Surface Chemistry

Adsorption

Surface tension, capillary action, pressure difference across curved surface (Laplace equation), vapour pressure of droplets (Kelvin equation), Gibbs adsorption isotherm, catalytic activity at surfaces estimation of surface area (BET equation), Surface catalysed oxidation of Co to CO_2 ,surface films on liquids Surface equation of state and its application, Electro-kinetic phenomenon.

Micelles

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

UNIT III

Electrochemistry

Electrochemistry of solutions. Debye-Huckel–Onsager treatment and its extension, ion solvent interactions. Deby-Huckel-Bjerrum model. Solution of Strong electrolytes. Debye-Huckel theory for activity coefficient of electrolytic solutions; determination of activity and activity coefficients; ionic strength.

Thermodynamics of electrified interface equations. Derivation of electro-capillarity, Lippmann equations (surface excess), methods of determination. Structure of electrified interfaces, Helmltoz-Perrin, Guoy–Champman, Stern models.

Over potentials, exchange current density, derivation of Butler– Volmer equation, Tafel plot.

Polarography theory, llkovic equation; half wave potential and its significance, Cyclic voltametry.

Introduction to corrosion, homogenous theory, forms of corrosion, corrosion monitoring and prevention methods.

Books Recommended

1. Physical Chemistry , P.W.Atkins and J. D. Paulo, Oxford, 2013, 10th edition New Delhi.
2. Physical Chemistry, T. Engel and P. Reid, Pearson, 2006, 1st edition, New Delhi.
3. Physical chemistry of the surfaces, A.W. Adamson and A.P. Gast, John Wiley, 6th edition, 1997, New York.
4. Adsorption and Catalysis, D.K. Chakraborty, 1st edition, 1992, Narosa, New Delhi.
5. Surfactants and Polymers in aqueous solution, Krister Holmberg, Bo J¨onsson, Bengt Kronberg and Bj¨orn Lindman, 2002, John Wiley, Sussex.
6. Surfactants and interfacial phenomena, M.J. Rosen,John Wilay, 2nd edition, New Jeresy.
7. Chemical Kinetics, K.J.Laidler, Mcgraw-Hill.
8. Kinetics and Mechanism of Chemical Transformations, J.Rajaraman and J.Kuriacose, McMillan.
9. Modern Electrochemistry Vol.I and Vol.II. J.O.M.Bockris and A.K.N.Reddy, Plenum, 3rd edition, 1997, London.
10. Fast Reaction – D.N.Hague
11. Chemical Kinetics and Dynamics–2nd Edn. , JISteinfild, J.S.Fransis Co, W.L.Hase , Beutic Hall (1999).
12. Physical Chemistry- G. K Vemulapalli
13. Physical Chemistry- George Woodbury, Brooks cole

CH 411: INORGANIC CHEMISTRY PRACTICAL-II

Full Marks-50

Objective: To introduce multistep inorganic synthesis, separation and estimation of different metals from mixture.

Outcome: Ensures the students to understand and have hands on experience to preparer inorganic (coordination) compounds in multi steps and acquire knowledge of separation of metals from mixture.

(a) Separation and estimation of metal ions in following binary mixture (Cu-Ni, Ni-Zn, Cu-Fe etc.) involving volumetric and/or gravimetric methods.

(b) Preparations

Preparation of following compounds and their studies by elemental, IR and electronic spectra measurements.

i. *cis*-$K[Cr(C_2O_4)_2(H_2O)_2]$
ii. *cis and trans*-$\{Co(en)_2Cl_2]Cl$
iii. $Mn(acac)_3$
iv. $K_3[Fe(C_2O_4)_3]$
v. $[Ni(NH_3)_6]Cl_2$
vi. $Ni(dmg)_2$
vii. Tris(thiourea) copper(I) complex
viii. Potassium tris-(oxalato)aluminate(III)
ix. Tetraaminecopper(II) sulphate
x. Preparation of N,N-bis-(salicyldehyde)ethylenediamine, $salenH_2$ and Co(Salen) complex and determination of O_2 absorption by Co(salen)[6].
xi. Preparation of copper glycine complex-cis and trans-bis(glycinato)copper(II)[7].

(c) Spectrophotometric Determinations

i. Manganese / Chromium / Vanadium in steel sample
ii. Iron-phenanthroline complex: Job's Method of continuous variations.

iii. Copper-ethylene diamine complex: Slope-ratio method.

(d) Flame Photometric Determinations

i. Sodium and potassium when present together

(e) **Nephelometric determinations**

i. Sulphate/Phosphate.

Books Recommended

1. Inorganic Experiments, J. Derck Woollins., 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. An Advanced Course of Practical Chemistry, Nad, Ghosal & Mahapatra, Central Publisher (2000).
5. Vogel's Qualitative Inorganic Analysis, 7th Ed, Revised by G. Svehela, 4th Ed., Person (2007).
6. J. Chem. Educ., 1977, 54, 443, 1973, 50,670; Acc. Chem. Res., 1975, 8, 384.
7. J. Chem. Soc Dalton, 1979, 1901. J. Chem. Edu.,1982, 59, 1052.

CH 412: ORGANIC CHEMISTRY PRACTICAL-II

Full Marks-50

Objective: To impart knowledge of art of organic synthesis.

Outcome: Upon completion of this course students will be able to understand the different reactivity pattern of different reagents, and understand how to synthesize different organic compounds.

Organic Synthesis

(a) Preparation of Anthranilic acid
(b) Preparation of Methyl Orange
(c) Preparation of Adipic acid by chromic acid oxidation of cyclohexanol.
(d) p-chloro toluene from p-toluidine (Sandmeyer reaction)
(e) Synthesis of p-nitroaniline & p-bromo aniline (Aromatic electrophilic substitution)
(f) Synthesis of triphenyl methanol from benzoic acid (Grignard reaction)

Quantitative Analysis

(a) Estimation of Anilines / Phenols using hromate bromide solution.
(b) Determination of Iodine and Saponification values of an oil sample.
(c) Determination of DO, COD & BOD of Water samples.

Books Recommended

1. Experiments and Techniques in Organic Chemistry, D.Pasto, C.Johnson, & M.Miller, Prantice Hall.
2. Systemetic Qualitative Organic Analysis, H.Middleton, Edward Arnold (Publisher).
3. Hand Book of Organic Analysis, Qualitative & Quantitative, M.T.Clarke, Edward Arnold (Publisher).
4. Vogel's Text Book of Practical Organic Chemistry, A.R. Tatchell, John Wiley.
5. Macroscale and Microscale Organic Experiments, K.L.Williamson, D.C.Heath.
6. A Text Book of Practical Organic Chemistry (Qualitative). Arthur I.Vogel.

CH 413: SPECTROSCOPY-II

Unit pattern

Mid Sem: 20 marks
End Sem: 50 marks

Objective: The course is designed to understand the nuclear and electron spin resonance spectroscopy in a fundamental way. It also contains vibrational and Raman spectroscopy. A thorough discussion on all basic principles and applications are being included.

Outcome: As it can be seen the spectroscopic techniques discussed are very routine and useful, it is essential every student must have exposure to the course, and by this they will be competent in explaining and solving most of chemical structure analysis.

UNIT I

Nuclear Magnetic Resonance Spectroscopy

Nuclear spin; nuclear resonance, saturation, shielding of magnetic nuclei, chemical shift and its measurements, factors influencing chemical shift, deshielding, spin-spin interactions, factors influencing coupling constant 'J'. Classification (ABX, AMX, ABC, A_2B_2 etc.), spin decoupling; basic ideas about instrument, NMR studies of nuclei other than proton–^{13}C, ^{19}F and ^{31}P. FT NMR, advantages of FT NMR, use of NMR in medical diagnostics.

UNIT II

Electron Spin Resonance Spectroscopy

Basic principles, zero field splitting and Kramer's degeneracy, factors affecting the 'g' value. Isotropic and anisotropic hyperfine coupling constants, spin Hamiltonian, spin densities and McConnell relationship, measurement techniques, applications.

Nuclear Quadrupole Resonance Spectroscopy

Quadrupole nuclei, quadrupole moments, electric field gradient, coupling constant, splittings, Applications.

UNIT III

Vibrational Spectroscopy

Infrared Spectroscopy

Review of linear harmonic oscillator, vibrational energies of diatomic molecules, zero point energy, force constant and bond strengths; anharmonicity, Morse potential energy diagram, vibration-rotation spectroscopy, P, Q, R branches. Born-Oppenheimer approximation, Breakdown of Oppenheimer approximation; vibrations of polyatomic molecules

Selection rules, normal modes of vibration, group frequencies, overtones, hot bands, factors affecting the band positions and intensities, far IR region, normal co-ordinate analysis.

Raman Spectroscopy

Classical and quantum theories of Raman effect. Pure rotational, vibrational and vibrational-rotational Raman spectra, selection rules, Mutual exclusion principle. Resonance Raman spectroscopy, coherent anti Stokes Raman spectroscopy (CARS).

Books Recommended

1. Modern Spectroscopy, J.M.Hollas, John Wiley, 4th edition, Sussex.
2. Applied Electron Spectroscopy for Chemical Analysis Ed. H. Windawi and F.L.Ho, Wiley Inter science.
3. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, R.V. Parish, Ellis Harwood, 1st edition, 1990.
4. Physical Methods in Chemistry, R.S.Drago, Sauders College.
5. Chemical Applications of Group Theory, F.A.Cotton.
6. Introduction to Molecular Spectroscopy, G.M.Barrow, McGraw Hill
7. Basic Principles of Spectroscopy, R.Chang, McGraw Hill.
8. Theory and Applications of UV Spectroscopy, H.H.Jaffe and M.Orchin, IBH-Oxford.
9. Introduction to Photoelectron Spectroscopy, P.K.Ghosh, John Wiley.
10. Introduction to Magnetic Resonance, A. Carrington and A.D. Maclachalan, Harper & Row.
11. Inorganic spectroscopic methods, A.K. Brisdon, Oxford Chem. Primers, 1997, New York.
12. Spectroscopy, S. Walker and H. Straw, Chapman and Hall ltd.

13. Energy levels in atom and molecules, W.G. Richards and P.R. Scott, Oxford, Oxford Chemistry Primer vol. 26, 1994, New York.
14. Introduction to Spectroscopy, Pavia, Brooks/Cole Cenage, 4th edition, 2009, Belmont.
15. EPR: Elemental theory and applications, J.A. Well. J.R. Bolton,Wiley, 2nd edition, 2007, New Jeresy.
16. Electron Paramagnetic resonance of transition ions, A. Abraham andB. Bleaney, Clarendon Press, 1970, Oxford.
17. Essentials of Nuclear Chemistry, H.J. Arnikar, John Wiley, 4th edition, 1995, New Delhi.
18. Fundamental of Molecular Spectroscopy, C. N. Banwell and E. McCash, Tata McGraw Hill, 4th edition, 1994, New Delhi.
19. Fundamental concept of Inorganic Chemistry- A.K. Das and Mahua Das, CBS Publisher
20. Symmetry and Spectroscopy of Molecules, , K.V. Reddy, New Age International (P) Ltd., Ist Ed.,, (1998).

CH 414: ANALYTICAL CHEMISTRY

Unit pattern

Mid Sem: 20 marks
End Sem: 50 marks

Objective:

1. To familiarize the students with some instrumental techniques of characterization of different sample.
2. To understand the basic/working principles, instrumentation, analysis of thermal and electrochemical methods.
3. To understand the basic/working principles and instrumentation of some spectroscopic techniques and their use in chemical analysis.

Outcome: At the end of the students will be able

1. Explain the theoretical basis of different analytical techniques with understanding on operational procedure.
2. Selection of appropriate analytic techniques for analysis of sample and interpretation of analytical results
3. Interference in different analytical techniques and their elimination

UNIT I

Thermal analysis

Thermogravimetric analysis (TGA): Instrumentation, derivative therogravimetric analysis (DTG), applications of thermagravimetry.
Differential Thermal Analysis (DTA): Principle, instrumentation and applications of differential thermal analysis, simultaneous TG-DTA curves.
Differential scanning calorimetry (DSC): Principle, basic instrumentation and applications.
Thermogravimetic titration: Principle and applications.

UNIT II

Electroanalytical methods

Classification of electroanalytical methods, principles and applications of voltammetry, cyclic voltaammetry, anodic stripping voltammetry, polarography, amperometry, coulometry, conductometry and ion selective electrodes (Extensive instrumentations are to be excluded).

UNIT III

Spectroscopic methods

Atomic adsorption spectroscopy: Principle and instrumentation, flame atomization, hollow cathode lamps, interference in AAS, applications of AAS in qualitative and quantitative analysis.

Flame photometric methods: Basic principle and instrumentation, interference in flame photometry, applications in quantitative analysis.

Nephhelometric method: Principle and instrumentation, applications in analysis.

Book Recommended

1. Fundamentals of Analytical Chemistry, D.A.Skoog, D.M.West and F.J.Hollar. 7th Edition, Harcourt College Publishers, 1996.
2. Analytical Chemistry, Gary D. Christian, 6th Edition, John Wiley & Sons (Aisa) Pte Ltd (Wiley Student Edn) 2004.
3. Introduction to thermal analysis: Techniques an application, M. E. Brown, Kluer Academic Publisher, New York (2004).
4. Instrumental Methods of Analysis, H.H.Williard. L.L.Merritt and J.A.Dean East-West press, New Delhi, 1988.
5. Principles and Practice of Analytical Chemistry, F.A. Fifield & Dacid Kealy, Blackwell Publishing, 5th Edn, 2000.
6. Analytical Chemistry (Theory and practice) U. N. Dash

SEMESTER-III

CH 501: PERICYCLIC REACTIONS AND PHOTOCHEMISTRY

Unit pattern

Mid Sem: 20 marks
End Sem: 50 marks

Objective: To impart knowledge of pericyclic reactions, photochemistry of alkene, carbonyl compounds and aromatic compounds.

Outcome: Upon completion of this course students will be able to understand the molecular origin of pericyclic reactions, understand the concept of interaction of organic compounds with light and subsequently trigger the reaction, understand the mechanism photochemistry of alkene, carbonyl compounds and aromatic compounds.

UNIT I

Pericyclic Reactions.

Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3 – butadiene, 1,3,5 – hexatriene and allyl system. Classification of pericyclic reactions. Woodward – Hoffmann correelation diagrams. FMO and PMO approach. Electrocyclic reactions – conrotatory and disrotatory motions, 4n, 4n+2 and allyl systems. Cycloadditions – antarafacial and suprafacial additions, 4n and 4n+2 systems, 2+2 addition of ketenes, 1,3 dipolar cycloadditions and cheleotropic reactions.

Sigmatropic rearrangements – suprafacial and antarafacial shifts of H, sigmatroic shifts involving carbon moieties, 3,3 – and 5,5 – sigmatropic rearrangements. Some variants of Claisen rearrangement (Johnson, Ireland, Abnormal, Asymmetric aromatic), Cope, and Aza-cope, Oxy-cope rearrangements. Fluxional tautomerism, Ene reaction

UNIT II

Photochemical Reactions

Interaction of electromagnetic radiation with matter, types of excitations, fate of excited molecule (singlet, triplet state), Jablonski diagram (fluorescence, phosphorescence, delayed fluorescence), Excimer, Exciplex, quantum yield/quantum efficiency, transfer of excitation energy (Sensitization & quenching), Actinometry. Types of photochemical reactions – photo-dissociation, gas-phase photolysis.

Photochemistry of alkenes

Intramolecular reactions of the olefinic bond – geometrical isomerism, cyclisation reactions, rearrangement of 1,4 – and 1,5 – dienes, Di-π methane rearrangement.

UNIT III

Photochemistry of Carbonyl Compounds

Intramolecular reactions of carbonyl compounds – saturated, cyclic and acylic, β,γ- unsaturated and α,β- unsaturated compounds, Norrish type I and II reaction, Paterno-Buechi Reaction, Cyclohexadienones, Photodimerisation of carbonyl compounds.

Photochemistry of Aromatic Compounds

Ring Isomerisations, additions, & substitutions, Cyclization reaction.

Miscellaneous Photochemical Reactions

Photo-Fries rearrangement, Photo-Fries reactions of anilides, Barton reaction. Singlet molecular oxygen reactions, Photochemical formation of smog, Photodegradation of polymers, Photochemistry of vision.

Book recommended:

1. Pericyclic Reactions, S. M. Mukherji, Macmillan, India.
2. Conversion of Orbital Symmetry, R.B. Woodward and R. Hoffman
3. Organic Reactions and Orbital Symmetry,R. C. Storr, T. L Gilchrist

4. Fundamentals of Photochemistry, K.K.Rohtagi-Mukherji, Wilcy-Eastern.
5. Molecular Photochemistry, N.J.Turro, W.a.Benjamin.
6. Introductory Photochemistry, A.Cox and T.Camp. McGraw-Hill.
7. Photochemistry, R.P.Kundall and A.Gibert, Thomson Nelson.
8. Organic Photochemistry, J.Coxon and B.Halton, Cambridge University Press.

CH 502: BIOINORGANIC & SUPRAMOLECULAR CHEMISTRY

Mid Sem: 20 marks
End Sem: 50 marks

Objective:

1. To study the role on the role of metals in biological systems and medicine.
2. To introduce the student on structure, stereochemistry and biological functions of different metalloenzymes.
3. To study the structure and function of biomolecules in nitrogen fixation and photosynthesis.
4. To introduce concept molecular recognition, interactions in supramolecular systems and their applications

Outcome: On completion of the course the student will

1. Understand and acquire knowledge of effect of deficiency and toxicity of metals in both human and plant systems.

2. Describe the structural and functional relationships, mechanisms and importance of metaloenzymes.
3. Understand the fundamentals of supramolecules, supramolecular reactions and catalysis, devises.

UNIT I

Metal ions in biological systems and its storage transport and biomineralization

Essential and trace elements, Ferritin, transferrin, and siderophores.

Calcium in Biology

Transported regulation, Intracellular Ca^{2+} transport, Ca^{2+}ATpase, Na^{+}/Ca^{2+} exchange, mitochondrial influx and efflux. Inositol triphosphate, Ca^{2+} regulated intracellular processes: Calmodulin, Troponin C,

Metalloenzymes

Zinc enzymes: Carboxypeptidase and carbonic anhydrase; Iron enzymes: catalase peroxidase and cytochromes, Cyt-P450; Copper enzymes: Superoxide dismutase; Molybdenum oxatransferase enzymes: xanthine oxidase. **Coenzyme** vitamin B_{12}. sulphur proteins

UNIT II

Nitrogen fixation

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

Photosynthesis

Chlorophylls, photo system I and photo system II in cleavage of water

Transport and storage of dioxygen

Heme proteins and oxygen uptake, structure and function of hemoglobin, myoglobin, hemocyanins and hemerthrin, model synthetic complexes of iron, cobalt and copper

UNIT III

Supramolecular Chemistry.

Concepts and language

(A) Molecular recognition: Molecular receptors for different types of molecules including anionic substrates, design and synthesis of coreceptor molecules and multiple recognition.
(B) Supramolecular reactivity and catalysis.
(C) Transport processes and carrier design.
(D) Supramolecular devices, supramolecular photochemistry, supramolecular electronic, ionic and switching devices.
Some example of self-assembly in supramolecular chemistry

Books Recommended

1. Principles of Bioinorganic Chemistry, S .J. Lippard and J. M. Berg., University Science Books.
2. Bioinorganic Chemistry, I. Bertini, H. B. Gray, S. J. Lippard and J. S. Valenting, University Science Books.
3. Inorganic Biochemistry vols I and II ed. G. L.Eichhom, Elsevier.
4. Progress in Inorganic Chemistry, Vols 18 and 38 ed, by J. J. Lippard, Wiley.
5. Bioinorganic Chemistry, Asim K. Das, Books and Allied, 2nd Ed., (2007).
6. Supramolecular Chemistry, J. W. Steed and J. L. Atwood, Willey, 2nd Ed., (2009).
7. Bioorganic, Bioinorganic and Supramolecular Chemistry, P. S. Kalsi, J. P. Kalsi, New Age International, 2nd Ed., (2012).
8. An Introduction of Supramolecular Chemistry, Asim K. Das, Books and Allied, 1st Ed., (2017).

CH 503: APPLIED CHEMISTRY PRACTICAL

Full Marks-50

Objective:

1. To familiar the student with the chemistry of synthesis of Nylon 6, 6 and other similar polymers,
2. To acquire a minimum practical skill to determine the molecular weight of polymers and thier characterization by other methods
3. To learn the conventional techniques of analysis of different water parameters and specific components in different samples by classical/instrumental methods.

Outcome: After the completion of course students will be able

1. To perform experiment on preparation of polymers and their basic characterizations.
2. To perform the analysis of different water parameters using classical and instrumental methods.
3. To understand the principles behind the experiment performed in the laboratory

Synthesis of polymers

i. Novalac/resole resin using phenol and formaldehyde.
ii. Polyethylene tetrasulphide by emulsion polymerization.
iii. Synthesis of Nylon 6,6

Characterisations of polymers

i. Determination of viscosity average molecular weight of polystyrene (PS), polyninyl alcohol (PVA), polyethyleneglycol (PEG), Polyacrylamide (PA).
ii. Thermal and spectral (IR) analysis of selected polymers

Analysis of water parameters

i. Determination of (i) Dissolved Oxygen (DO), (ii) Chemical Oxygen Demand (COD) and (iii) Biochemical Oxygen Demand (BOD) in water samples.
ii. Analysis of a ground water sample for sulphate by titrimetry (EDTA) and turbidimetry.
iii. Determination of fluoride in drinking water/ground water by spectrophotometry (alizarin red lake method).
iv. phosphate by molybdenum blue method

Miscellaneous

i. Spectrophotometric estimation of phosphate in cola drinks
ii. Analysis of fat in a butter sample
iii. Spectrophotometric estimation of hexavalent chromium in water samples.
iv. Determination of ascorbic acid in vitamin C tablets.
v. Verification of Beer's Lambart law

Flame photometry

Determination of Na^+ / K^+ ions in water sample/soil by flame photometry

Books Recommended.

1. Vogel's Text Book of Quantitative Chemical Analysis By J.Mendham, R.C.Denney, J.D.Barnes, M.J.K. Thomas, Pearson Education Publishers, 6thy Edition.
2. Hand book of Environmental analysis by Pradyot Patnaik, Lewis Publishers, USA (1997).
3. Standard Methods for the Examination of Water and Wastewater, APHA, AWWA, WPCF, Washington, DC, USA, 17th Edition.

CH 504: PHYSICAL CHEMISTRY PRACTICAL-I

Full Marks-50

Objective:

The laboratory course is framed on the basis of instruments such as conductivity meter, pH meter and potentiometer, where a number of experiments based on conductivity measurement, pH measurement and potential measurement can be performed.

Outcome:

It is believed that students performing the experiments will be capable of handling the conductivity meter, pH meter and potentiometer. Also it gives a real feel of the electrochemistry, such a verification of Debye-Huckel-Onsager equation, neutralisation of weak acids, determination of K_{sp} of sparingly soluble salt and conductometric titrations, which are taught in theory.

Error Analysis and Statistical Data Analysis

Errors, types of errors, minimization of errors, error distribution curves, precision, accuracy and combination; statistical treatment for error analysis, student 't' test, null hypothesis, rejection criteria, F & Q test; linear regression analysis, curve fitting.

Calibration of volumetric apparatus, burette, pipette and standard flask.

Adsorption

To study surface tension – concentration relationship for solutions (Gibbs equation)

Chemical Kinetics

(i) Determination of the effect of (a) Change of temperature (b) Change of concentration of reactants and catalyst and (c) Ionic strength of the media on the velocity constant of hydrolysis of an ester / ionic reactions.

(ii) Determination of the velocity constant of hydrolysis of an ester / ionic reaction in micellar media.

(iii) Determination of the rate constant for the oxidation of iodide ions by hydrogen peroxide studying the kinetics as an iodine clock reaction.

Solutions

(i) Determination of the degree of dissociation of weak electrolyte and to study the deviation from ideal behaviour that occurs with a strong electrolyte.

Electrochemistry

A. Conductometry:

(i) Determination of the velocity constant, order of the reaction and energy of activation for saponification of ethyl acetate by sodium hydroxide conductometrically.

(ii) Determination of solubility and solubility product of sparingly soluble (e.g., $PbSO_4$, $BaSO_4$) conductometrically.

(iii) Determination of the strength of strong and weak acids in a given mixture conductometrically.

(iv) Determination of the activity coefficient of zinc ions in the solution of 0.002 M zinc sulphate using Debye Huckel's limiting law.

B. Potentiometry / pH metry:

(i) Determination of strengths of halides in a mixture potentionmetrically.

(ii) Determination of the valency of mercurous ions potentiometerically.

(iii) Determination of the strength of strong and weak acids in a given mixture using a potentiometer / pH meter.

(iv) Acid-base titration in a non-aqueous media using a pH meter.

(v) Determination of the dissociation constant of acetic acid in acetone by titrating it with KOH in what medium.

(vi) Determine the PK's of a dibasic acid by pH titration using a pH meter.

C. Polarimetry

(i) Determination of rate constant for hydrolysis / inversion of sugar using a polarimeter.
(ii) Enzyme kinetics – inversion of sucrose.

Books Recommended

1. Practical Physical Chemistry, A. M. James and F.E. Prichard, Longman.
2. Findley's Practical Physical Chemistry, B. P. Levitt, Longman.
3. Experimental Physical Chemistry, R. C. Das and B. Behera, Tata McGraw Hill, 1983, New Delhi.
4. Vogel's Text book of Quantitative Analysis, revised, J.Bassett, R.C.Denney, G.H. Jeffery and J.Mendham, ELBS.
5. Fundamentals of Analytical Chemistry, D.A.Skoog, D.M.West and F.J.Hollar. 7th Edition, Harcourt College Publishers, 1996.

CH 505: APPLICATION OF SPECTROSCOPY-I

Unit pattern

Mid Sem: 20 marks
End Sem: 50 marks

Objective: The course content is aimed at providing a very basic entry into the subject of shift reagents, in particular the influence of paramagnetic substances on a NMR signal. It also attempts to introduce a student in the field of NMR of metalloenzymes. Mössbauer spectroscopy is a versatile technique that can be used to provide information about the chemical bonding, chemical structural, oxidation states of a material. It is a useful technique involving gamma ray spectroscopy

Outcome: The discussion on the course content is definitely beneficial in terms of a student getting idea of NMR of biomolecules and the application of shift/contrast reagents, used in MRI studies. Further, students will understand a Mössbauer spectrum, understand the concept of chemical shift, determine oxidation state, electric quadrapole interaction, determines the chemical structure and bonding, hyperfine interactions.

UNIT I

Vibrational Spectroscopy

Normal modes of vibration, Determination of normal modes from Symmetry for AB_2, AB_3, AB_4, AB_5 and AB_6 systems, symmetry of overtones and combination bands, mode of bonding of ambidentate ligands, ethylenediamine and diketonato complexes, application of ir spectra to complexes, Resonance Raman Spectroscopy and its application , particularly for the study of active sites of metallo-proteins myoglobin and hemoglobin.

UNIT II

Spin Resonance Spectroscopy

Electron Spin Resonance Spectroscopy

Hyperfine coupling, spin polarization for atoms and transition metal ions, spin-orbit coupling and significance of g-tensors, applications to transition metal complexes (having one unpaired electron) including biological systems and to inorganic free radicals such as PH_4, F_2 and $[BH_3]^-$ etc.

Nuclear Magnetic Resonance of Paramagnetic Substances in solution

The contact and pseudo contact shifts, factors affecting nuclear relaxation, some applications including biochemical systems, an overview of NMR of metal nuclides with emphasis of ^{195}Pt and ^{119}Sn NMR.

UNIT III

Mossbauer Spectroscopy

Basic principles, spectral line shape and natural line width, characteristics of Mossbauer nucleides, Dopplers effect, Mossbauer spectra of ^{57}Fe system, Mossbauer spectra of ^{119} Sn system, parameters to evaluate Mossbauer spectra : chemical shift or isomeric shift, qudrapole interaction, Magnetic field interaction. Application of the technique to the studies of (1) bonding and structures of Fe^{+2} and Fe^{+3} compounds including those of intermediate spin, Sn^{+2} and Sn^{+4} compounds, nature of M-L bond, structure and detection of oxidation state and inequivalent MB atoms.

Books recommended:

1. Physical Methods for Chemistry, R.S.Drago, Saunders Company.
2. Structural Methods in Inorganic Chemistry, E.A.V.Ebsworth, D.W.H.Rankin and S.Cradock, ELBS.
3. Infrared and Raman Spectra: 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_1 R.L. Carlin Vol.3, Dekker
7. Inorganic Electronic Spectroscopy, A.P.B.Lever, Elsevier
8. Practical NMR Spectroscopy, M.L.Martin, J.J.Delpeuch and G.J.Martin, Heyden. A. Gibert, Thomson Nelson.
9. Organic Photochemistry, J.Coxon and B.Halton, Cambridge University Press.
10. Introduction to Spectroscopy, Pavia, Brooks/Cole Cenage, 4th edition, 2009, Belmont.
11. EPR: Elemental theory and applications, J.A. Well. J.R. Bolton,Wiley, 2nd edition, 2007, New Jeresy.
12. Electron Paramagnetic resonance of transition ions, A. Abraham andB. Bleaney, Clarendon Press, 1970, Oxford.
13. Essentials of Nuclear Chemistry, H.J. Arnikar, John Wiley, 4th edition, 1995, New Delhi.
14. Fundamental of Molecular Spectroscopy, C. N. Banwell and E. McCash, Tata McGraw Hill, 4th edition, 1994, New Delhi.
15. B.M. Still, P.G. Anil Kumar, J.R. Aldrich-Wright, W.S. Price, Chem. Soc. Rev. 36 (2007) 665.
16. Mossbauer spectroscopy- Greenwood and Gibbs
17. Mossbauer spectroscopy and transition metal Chemistry-m Gutlich, Link, Trautween
18. Fundamental concept of inorganic chemistry, Vol-7- A.K.Das and Mahua Das, CBS Publisher
19. Molecular structure and Spectroscopy- Aruldhas
20. Analytical chemistry – Theory and practice- U.N.Das

CH 506: ORGANIC SYNTHESIS

Unit pattern

Mid Sem: 20 marks
End Sem: 50 marks

Objective: To impart knowledge of oxidation and reduction, protection of alcohol, amine, carbonyl and carboxyl compounds and disconnection approach in synthesis of various natural products.

Outcome: Upon completion of this course students will be able to understand the philosophy of synthesis of various natural products, understand the reactivity pattern and underlying reaction mechanism of different oxidizing and reducing reagents, and understand the art of selective protection and deprotection of alcohol, amine, carbonyl and carboxyl groups in organic compounds.

UNIT I

Oxidation

Oxidation of organic molecules using Ruthenium tetraoxide, Hypervalent iodine, thallium(III)nitrate, Dichlorodicyano benzoquinone (DDQ), Selenium dioxide, Dimethyl sulfoxide, Peracids, Oxone, Dioxiranes, Tetramethyl piperidine nitroxide, Singlet oxygen, Ozone, N-sulfonyl oxaziridine, Chromium Manganese, Silver, Ruthenium, Osmium, Molybdenum, Lead, Mercury based reagents. Suzuki coupling, Negishi coupling, Stille coupling, Heck Reaction

Reduction

Reduction of organic molecules using Boron based reagents, Aluminum-based reagents, Free radical reagent, Silane based reagents, Dissolving metal reduction, Diimide reduction, Wolff-Kishner reduction, Hydrogenation using Pd, Pt, Rh, Ni on solid support.

UNIT II

Protecting Groups

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

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 reactions, amine synthesis.

One Group C-C Disconnection

Alcohols and carbonyl compounds, regioselectivity, Alkene synthesis, use of acetylenes and aliphatic nitro compounds in organic synthesis.

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.

Ring Synthesis

Saturated heterocycles, synthesis of 3-, 4-, 5- and 6-membered rings, aromatic heterocycles in organic synthesis

UNIT III

Synthesis of some Complex Molecules

Application of the above in the synthesis of following compounds. Camphor, Longifoline, Cortisone, Reserpine, prostaglandin, Juvabione, Aphidicolin and Fredericamycin A.

Books Recommended

1. Designing Organic Synthesis, A programmed introduction to synthon approach, S. Warren, Wiley.
2. Organic Synthesis-Concept, Methods and Starting Materials, J.Fuhrhop and G.Penzillin, VCH, Weinheim, Germany.
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 Streucture, J.March, Wiley.
6. Principles of Organic synthesis, R. Norman and J.M. Coxon, Blackie Academic & Professional.
7. Advanced Organic Chemistry Part B, F.A. Carey and R.J.Sundberg, Plenum Press.

8. Organic Chemistry: The disconnection approach, S. Warren, John Wiley and Sons.

CH 507: ENVIRONMENTAL CHEMISTRY
Unit pattern

Mid Sem: 20 marks
End Sem: 50 marks

Objective: To acquaint the student with a basic understanding of the concept and structure of environment, about the chemical composition of the different matrices of the environment (air, water, soil) and the interaction involved between them, understand different types of air, water, soil and radiation pollution and its consequences, different steps of waste management, to study about different industrial effluents, pollution by industry and their remedies, global environmental issues and disasters, and green solution to environmental problems.

Outcome: After the completion of course students will able to describe the structure and significance of the spheres of the environment, the important environmental issues and the factors responsible for their cause, understand the significance of environmental science as a subject, explain the chemical nature and interaction of the air, water and soil, apply analytical tools to determine and measure pollutants in various environmental samples, explain environmental pollution issues and the remedies thereof, and understand about green chemistry principles and their applications.

UNIT I

Environment

Introduction, Composition of atmosphere, vertical temperature, heat budget of the earth atmospheric system, vertical stability atmosphere. Biogeochemical cycles of C, N, P, S and O. Biodistribution of elements.

Hydrosphere

Chemical composition of water bodies: lakes, streams, rivers and wet lands etc. Hydrological cycle.

Aquatic pollution-inorganic, organic, pesticide, agricultural, industrial and sewage, detergents, oil spills and oil pollutants. Water quality parameters- dissolved oxygen, biochemical oxygen demand, solids, metalsm, content of chloride, sulphate, phosphate, nitrate and micro-organisms. Water quality standards

Analytical methods for measuring BOD, DO, COD, F, Oils, metals (As, Cd, Cr, Hg, Pb, Se etc.) residual chloride and chlorine demand.

Purification and treatment of water.

UNIT II

Soils

Composition, micro and macro nutrients, Pollution –fertilizers, pesticides, plastics and metals. Waste treatment.

Atmosphere

Chemical composition of atmosphere-particles, ions and radicals and their formation. Chemical and photochemical reactions in atmosphere, smog formation, oxides of N, C, S, O and their effect, pollution by chemicals, petroleum, minerals, chlorofluorophydrocarbons. Green house effect, acid rain, air pollution controls and their chemistry.

Analytical methods for measuring air pollutants. Continuous monitoring instruments.

UNIT III

Industrial Pollution

Pollution obtained due to Cement, sugar, distillery, drug, paper and pulp, thermal power plants, nuclear power plants, metallurgy , Polymers, drugs etc. industry and steps to reduce

pollution. Radionuclide analysis. Solid waste management. Disposal of wastes and their management.

Environmental Toxicology

Chemical solutions to environmental problems, biodegradability, principles of decomposition better.

Books Recommended

1. Environmental Chemistry , S.E. Manahan, Lewis Publishers
2. Environmental Chemistry, A.K. De, Wiley Eastern.
3. Environmental Chemistry with Green Chemistry, A. K. Das, Books & Allied (P) Ltd., Kolkata, 1st Edn, 2010.
4. Environmental Toxicology, Ed. J. Rose, Gordon and Breach Science Publication, Elemental Analysis of Airborne Particles, Ed. S. Landsberger and M. Creatchman, Gordon and Breach Science Publication.
5. Environmental Chemistry, C. Baird, W.H. Freeman
6. Hand Book of Environmental Analysis, Pradyot Patnaik, Lewis Publishers (1997)
7. Standard Methods for the Examination of Water and Wastewater, APHA, AWWA, WPCF, Washington D.C. 20005, USA, 17th Edition (1998)

CH ADD1: TECHNIQUES OF CHEMICAL ANALYSIS

Unit pattern

Mid Sem: 20 marks
End Sem: 50 marks

Objective: Chemical analysis is conducted for a wide range of purposes from material identification and characterization to quality control monitoring. The aim of this course is to provide students with a broad understanding of the methods of chemical analysis and their applications in analyses of different kinds of samples.

Outcome: At the end of the course, student will be able to explain the principle of different methods of chemical analysis applicable to different types of samples, select and apply the appropriate analytical method for chemical analysis of a specific sample, and interpret the qualitative and quantitative results of analysis.

Unit-I

Introduction to various methods of chemical analysis. Classical and instrumental methods of chemical analysis, selection of analytical methods, methods of sampling. Errors in chemical analysis and their minimisation.

Wet chemical analyses of minerals (iron ore and dolomite), soil and water.

Unit-II

Elemental Analysis: Detection, Identification, and Quantification. Different techniques of elemental analyses. Elemental analysers: Principle and applications for analysis of organic compounds.

Instrumental methods-I: UV-Visible Spectroscopy: Principle, instrumentation and chemical analysis of different samples.

Instrumental Methods-II: Atomic Absorption Spectroscopy (AAS), Inductively coupled Plasma (ICP) Spectroscopy, Flame photometry: Principle, instrumentation and applications with reference to chemical analyses of different samples.

Unit-III Chromatographic methods: Introduction & classification of chromatography. Principle, instrumentation (Exhaustive instrumentation are to be excluded) & applications of

(i) Column/Thin layer/Paper chromatography (ii) Ion chromatography (iv) Gas chromatography with special reference to chemical analyses.

Reference Books:

1. Fundamentals of Analytical Chemistry, D. A. Skoog and D. M. West and F. J Holler, Cengage, 9th edition, 2014
2. Instrumental Methods of Analysis, B. K. Sharma, Goel Publishing house
3. Chemical Analysis: Modern Instrumental Methods and Techniques, Rouessac, F; Rouessac, A; Wiley-Blackwell, 2000.
4. A Textbook of Quantitative Inorganic Analysis. Vogel, A.I. (1961) 3rd Edition, Longmans, 539

SEMESTER-IV

CH 508: BIOORGANIC CHEMISTRY

Unit pattern

Mid Sem: 20 marks
End Sem: 50 marks

Objective: To impart knowledge of biological catalysts, mechanism of enzyme action and reactions catalyzed by enzymes and co-enzyme.

Outcome: Upon completion of this course students will be able to understand how enzyme catalyzes the reaction with outmost efficiency, acid-base catalysis and covalent catalysis of enzyme, strain and distortion during enzyme catalysis, structure and biological functions of various coenzymes, and the origin of mechanism of enzyme action.

UNIT I

Introduction

Basic considerations Proximity effects and molecular Adaptation.

Enzymes

Introduction and historical perspective, chemical and biological catalysis, remarkable properties of enzymes like catalytic power, specificity and regulation. Nomeclature and classification, extraction and purification. Fischer's lock and key and Koshland's induced fit hypothesis, concept and identification of active site by the use of inhibitors, affinity labeling and enzyme modification by site-directed mutagenesis.

UNIT II

Mechanism of Enzyme Action

Kinetics of enzyme action, Michealis Menten and Lineweaver-Burk plots, revcersible and irreversible inhibition. Transition-state theory, orientation and steric effect, acid-base catalysis, covalent catalysis, strain or distortion. Examples of some typical enzyme mechanism for chymotrypsin, ribonuclease, lysozyme and carboxypeptidase A.

UNIT III

Reactions Catalyzed by Enzymes and Co-Enzyme Chemistry

Nucleophilic displacement on a phosphorus atom, multiple displacement reactions and the coupling of ATP cleavage to endergonic processes. Transfer of sulphate, addition and elimination reactions, enolic intermediates in isomerization reactions, β-cleavage and condensation, some isomerization and rearrangement reactions. Enzyme catalyzed carboxylation and decarboxylation. Cofactors as derived from vitamins, coenzymes, prosthetic groups, apoenzymes. Structure and biological functions of coenzyme. A, thiamine pyrophosphate, pyridoxal phosphate, NAD^+, $NADP^+$, FMN, FAD, lipoic acid, vitamin B_{12} Mechanisms of reactions catalyzed by the above cofactors.

Books Recommended

1. Biorganic Chemistry, A Chemical Approach to Enzyme Action, Hermann Dugas and C. Penny, Springer-Verlag.
2. Understanding Enzymes, Trevor Palmer, Prentice Hall.
3. Enzyme Chemistry: Impact and Applications, Ed. Collin J. Suckling, Chapman and Hall.
4. Enzyme Mechanisms Ed, M.I.Page and A. Williams, Royal Society of Chemistry.
5. Fundamentals of Enzymes: An Introduction and Applications in Biotechnology, Michael D. Trevan, John Wiley.
6. Immobilized Enzymes: An Introduction and Applications in Biotechnology, Michael D. Trevan, John Wiley.
7. Enzymatic Reaction Mechanisms C. Walsh, W.H.Freemain.
8. Enzyme Structure and Mechanism, A Fersht. W.H.Freeman.
9. Biochemistry: The Chemical Reactions of Living Cells, D.F.Metzler, Academic Press.

CH 509: ORGANOTRANSITION METAL CHEMISTRY

Mid Sem: 20 marks
End Sem: 50 marks

Objective:

1. To introduce the students on preparations, structure and bonding aspects of simple organometallic compounds
2. To study the methods of synthesis, properties and reactivity of organometallic compounds with metal-carbon multiple bonds.
3. To introduce on types of common organometallic reactions and mechanistic study of some homogeneous catalytic reaction systems involving organometallic compounds
4. To study the concept of fluxionality in organometallic compounds

Outcome: On completion of this course, the student will be able to

1. Describe the structure and bonding aspects of different organotransition metal compounds and their correlations with the stability and reactivity of such compounds.
2. Identify the different types of organotranstion metal complexes catalyzed reactions and explain mechanistic pathways of different catalytic reactions.
3. Describe the important applications of organometallic homogeneous catalysis in the production of organic chemicals**.**

UNIT I

Alkyl and Aryls of Transition Metals

Types, routes of synthesis, Stability and decomposition pathways organo- copper in organic synthesis

Compounds of Transition Metal-Carbon Multiple Bonds

Alkylidenes, Alkylidynes, low valent carbenes and carbynes-synthesis, nature of bond, structural characteristics, nucleophilic and electrophilic reactions on the ligands, role in organic synthesis.

UNIT II

Transition Metal π- Complexes

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

Transition Metal Compounds with Bonds to Hydrogen

Transition metal hydrides: Synthesis, properties and reactivity. Transition metal dihydrogen compound: Preparation, properties and reactivity.

UNIT III

Homogenous catalysis by Transition Metal Complexes

Coordinative unsaturation, oxidative addition and reductive elimination reactions. Insertion reactions (insertion of CO, SO_2 and alkenes). Reactions of coordinated CO in metal carbonyls. Homogenous hydrogenation of alkenes, hydroformylation of alkenes, isomerisation of olefins, Wacker's process, Zeigler-Natta Polymerization of ethylene, Monsanto acetic acid, Reduction of CO by hydrogen (Fischer-Tropsch reaction).

Fluxional Organometallic Compounds

Fluxionality and dynamic equilibria in compounds such as η^{2-} olefin, η^{3-} allyl and dienyl complexes.

Books Recommended

1. Principles and Application of Organotransition Metal Chemistry, J. P. Collman, L.S. Hegedus, J.R. Norton and R.G. Finke, University Science Books.

2. The Organometallic Chemistry of the Transition Metals, R .H. Carbtree, John Wiley.
3. Metallo-organic Chemistry, A.J.Pearson, Wiley.
4. The Organometallic Chemistry of the Transition Metals, R.H. Crabtree, 4th Ed, Willey (2005).
5. Fundamental Concepts of Inorganic Chemistry, Vol. 6; Asim K. Das, CBS Publisher, 2nd Ed., (2013).
6. Organometallic Chemistry, R.C. Mehrotra & A. Singh, New Age International, 2nd Ed (2013).

CH 510: POLYMER CHEMISTRY
Unit pattern

Mid Sem: 20 marks
End Sem: 50 marks

Objective: To study the fundamental concepts of polymer chemistry, structure of monomers, functionality, and classification of polymers on the basis of source, composition, conditions, molecular weight, geometry, industrial polymer fabrication process, and nomenclature of polymers.

Outcome: After the completion of course students will able to understand about the basics of polymer and the differences between crystalline melting temperature and glass transition temperature, as well as the effect of kinetics on both, develop specific skills, competencies, and thought processes sufficient to support further study or work in this field of polymer chemistry, evaluate the effect of factors such as polymer structure, molecular weight, branching and diluents on crystallinity, and apply knowledge to build up small scale industry for developing endogenous plastic product.

UNIT I

Basics

Importance of Polymers Basic concepts: Monomers, repeat units, degree of polymerization, Linear, branched and network polymers. Classification of Polymers. Polymerization Process-Condensation, Addition, Radical chain, Ionic and Co-ordination and Co-polymerization. Polymerization conditions and polymer reactions. Polymerization in homogeneous and heterogeneous systems.

Polymer Characterization methods

Polydispersion-average molecular weight concept. Number, weight and viscocity average molecular weights. Polydispersity and molecular weight distribution. The practical significance of molecular weight. Measurement of molecular weights-End-group, viscosity, light scattering, osmotic and ultracentrifugation methods. Analysis and testing of polymers-chemical analysis of polymers, spectroscopic methods: IR, UV, X-ray diffraction. Microscopic analysis: optical, SEM, and TEM. Thermal analysis- TGA, DSC, DTA, DMA and Physical testing-Tensile strength, Flexural strength, Fatigue, Impact strength, Tear resistance, Hardness and Abrasion resistance.

UNIT II

Structure, morphology and properties of polymer

Morphology and order in crystalline polymers-configurations of polymer chains. Crystal structures of polymers- Crystalline, Amorphous structure. Factors affecting crystallinity, degree of crystallinity, techniques to determine the degree of crystallinity, morphology of crystalline polymer, strain induced morphology, properties affected by crystallinity, Glass transition temperature: effects of molecular weight, diluents, chemical structure, chain topology, branching and cross linking on glass transition temperature. Tm-melting points of

homogeneous services: effect of chain flexibility, steric factor, entropy, and heat of fusion on Tm. Relation between Tg and Tm, Property requirements and polymer utilization.

UNIT III

Polymer Processing

Plastics, elastomers, and fibers. Resin, Compounding, Additives (crosslinking agent, UV stabilizer, fire retardant, coloring agent, plasticizer, and others). Processing techniques: Calendaring, die casting, rotational casting, film casting, injection molding, blow molding, extrusion molding, reinforcing, pultrusion and fiber spinning.

Properties of Commercial Polymers

Polythylene, polyvinyl chloride, polyamides, polyesters, phenolic resins, epoxy resins and silicone polymers. Functional polymers – Fire retarding polymers and electrically conducting polymers (PANI, Polyacetylene). Polymer in Biomedical applications: contact lens, dental polymers, artificial heart, kidney, skin, and blood cells.

Books Recommended

1. Text book of Polymer Science, F.W. Billmeyer, Jr.Wiley.
2. Polymer Science, V.R. Gowariker, N.V. Viswanathan and J. Sreedhar, Wiley-Eastern.
3. Functional Monomers and Polymers, K. Takemoto, Y. Inaki and R.M. Ottanbrite.
4. Contemporary Polymer Chemistry, H.R. Alcock and F.W. Lambe, Prentice Hall.

CH 511: SOLID STATE CHEMISTRY

Unit pattern

Mid Sem: 20 marks
End Sem: 50 marks

Objective: To obtain the knowledge on understanding solid state reactions, chemical synthesis methods, the structure of solids and crystal defects, insight into electronic structure and properties of crystals. These portions of solid state chemistry involves to introduction of optical and magnetic properties of solids, with basic understanding of several physical concepts such as optical reflectance, optical refraction and magnetic hysteresis. Also it gives an account of the generation of X-ray radiation and its effects of on matter. It includes neutron diffraction with a basic understanding of neutron properties and their utility in analysis of soft materials.

Outcome: Students will learn the structure, properties and the synthesis of solid materials. More significantly, crystal defects, electronic properties of solid can be easily explained. Also it will enable the student to interpret of crystal structure by X-ray diffraction and neutron diffraction method. After going through the course, it is believed that the student will be self-confident to explain certain optical and magnetic properties of solid state materials.

UNIT I

Solid State Reactions

General principles, experimental procedures, co-precipitation as a precursor to solid state reactions, sol-gel method

Crystal Defects and Non-Stoichiometry

Perfect and imperfect crystals, intrinsic and extrinsic defects–point defects- vacancies Schottky defects and Frenkel defects. Thermodynamics of Schottky and Frenkel defect formation, colour centres, non-stoichiometry defects, line defect- edge dislocation and Screw Dislocation and Plane defects- Grain boundaries, Tilt boundaries ,

Electronic Properties of solids

Metals, insulators and semiconductors, electronic structure of solids- Band theory, band structure of metals, insulators and semiconductors. Intrinsic and extrinsic semiconductors,

doping semiconductors, p-n junctions , super conductors (Low temperature superconductor, BCS theory, High temperature superconductor) .

UNIT II

Optical properties of solids

Optical reflectance, photoconduction-photoelectric effects, refraction, dispersion, polarization.

Magnetic Properties of Solids

Classification of materials. Quantum theory of paramagnetics – cooperative phenomena – magnetic domains, hysteresius.

Organic Solids

Electrically conducting solids, organic charge transfer complex, organic metals, new superconductors.

UNIT III

Diffraction Methods

X-ray Diffraction

Generation of X-rays, Properties of X-rays: continous spectrum, characteristic spectrum, Filters, Bragg condition, Miller indices, Structure factor and its relation to intensity, identification of unit cells from systematic absences in diffraction pattern. Structure factor calculation for NaCl, KCl,

Description of the procedure for an X-ray structure analysis, Laue method, Bragg method, Debye-Scherrer method of X-ray structural analysis of crystals, indexing of crystals,

Ramchandran diagram or [φ,ψ] plot.

Neutron Diffraction

Scattering of neutrons by solids and liquids, magnetic scattering, measurement techniques. Elucidation of structure of magnetically ordered unit cell.

Books Recommended

1. Solid State Chemistry and its Applications, A.R.West, Wiley, 1989, Singapore. 2nd Ed.,, Singapore.
2. Principles of the Solid State, H.V.Keer, Wiley Eastern, 1993, New Delhi
3. Solid State Chemistry, N.B. Hannay.
4. Solid State Chemistry, D.K. Chakrabarty, New Age International., 1996, New Delhi
5. Understanding solids, The Science of Materials, R. J. Tilley, John Wiley & Sons, 2004, Sussex.
6. Solid state Physics, Aschroft and Mermin, Harcourt College Press, 1976, Florida.
7. Solid state Physics, J.P. Srivastava.
8. Applications of neutron Powder diffraction, Kisi and Howard, Oxford Science, 2008, New York.
9. Elements Of X Ray Diffraction, B. D Cullity, Addison-Wesley Publishing Company Inc., 1956, USA.
10. Chemistry of solids: A.K. Galwey., Science paperbacks and Chapman and Hall Ltd.

CH 512: PHYSICAL CHEMISTRY PRACTICAL-II

Full Mark-50

Objective: The laboratory course is designed based on UV Visible spectrophotometer. Experiments such as determination of indicator constant, stoichiometry of a metal complex by Job's method are included.

Outcome: The conduct of these experiments will enable a student to understand Beer-Lambert's law in a better manner also the handling of an instrument will be learnt.

1. Thermodynamics

(i) Determination of partial molar volume of solute (e.g.,KCL) and solvent in a binary mixture.

(ii) Determination of the temperature dependence of the solubility of a compound in two solvents having similar intermolecular interactions (benzoic acid in water and in DMSO-water mixture) and calculate the partial molar heat of solution.

2. Spectroscopy

(i) Determination of pKa of an indicator (e.g., methyl red) in (a) aqueous and (b) micellar media.

(ii) Determination of stoichiometry and stability constant of inorganic (e.g. ferric – salicyclic acid) and organic (e.g. amine-iodine) complexes.

3. Polarography

(i) Estimation of Pb^{2+} and Cd^{2+} / Zn^{+} and Ni^{2+} ions in a mixture of Pb^{2+} and Cd^{2+} / Zn^{+} and Ni^{2+} by polarography.

(ii) Determination of dissolved oxygen in aqueous solution of organic solvents.

4. Electronics

This lab course will have theory as well as practicals and the lectures shall be delivered during lab hours.

5. Basic Electronics

Notations used in an electric circuit, study of electronic components and colour codes, conversion of chemical quantities into electrical quantities. Transducer, illustration with electrodes, thermocouples and thermistors.

6. Active Components

Introduction to ordinary diodes and Zener diodes with some emphasis on p-n juction as a solid state property. Use of diodes as rectifiers, clipping and clamping circuits. Power supplies.

Books Recommended

1. Experimental Physical Chemistry, B.P. Levitt, Longman.
2. Findlay's Practical Physical Chemistry, revised B.P. Levitt, Longman.
3. Experiments in Physical Chemistry, J.C.Ghosh, Bharati Bhavan.
4. Experimental Physical Chemistry, R.C. Behera and B. Behera, Tata McGraw Hill, 1983. New Delhi.

CH 513: PROJECT WORK

Full Mark-50

Objective: Students will research or review articles in a particular topic

1. To train the student to design experiment oriented project on particular context
2. To search literature on the selected topic of project work
3. To conduct the experiments scientifically as per selected topic and analyse the data
4. To develop the art of wiring the project report with proper citation of literature, data analysis, and presentation

Outcome: After completion of the project work the students will

1. Learn the design the experimental set up and perform the experimental as per specific problem selected for project
2. Gain the knowledge and competency to search literature and write the dissertation
3. Learn the skill for presentation of the project work.

Each student is required to submit dissertation of project work before theory examination for evaluation.

CH 514: APPLICATION OF SPECTROSCOPY-II
Unit Pattern

Mid Sem: 20 marks
End Sem: 50 marks

Objective: To impart knowledge of different spectroscopic technique for structural elucidation of organic compounds.

Outcome: Upon completion of this course students will be able to understand how Ultraviolet and Visible Spectroscopy, Infrared Spectroscopy, Nuclear Magnetic Resonance Spectroscopy and Mass Spectrometry are powerful technique to analyze the structural details of organic compounds, and predict different unknown compound based on UV-Vis, IR, ^{1}HNMR, ^{13}CNMR and mass spectroscopic data.

UNIT I

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 polynes Fleser-Woodward rules for conjugated dienes and carbonyl compounds, ultraviolet spectra of aromatic and heterocyclic compounds. Steric effect in biphenyls.

Infrared Spectroscopy

Instrumentation and sample handling, Characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols ethers, phenols and amines. Detailed study of vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters, amides, acids, anhydrides, lactones, lactams and conjugatged carbonyl compounds) Effect of hydrogen bonding and solvent effect on vibrational frequencies, overtones, combination bands and Fermi resonance, FTIR.

IR of gaseous, solids and polymeric materials.

Optical Rotatory Dispersion (ORD) and Circular Dichroism(CD).

Definition, deduction of absolute configuration, octant rule for ketones.

UNIT II

Nuclear Magnetic Resonance Spectroscopy

Chemical shift values and correlation for protons bonded to carbon (Aliphatic, olefinic, aldehydic and aromatic) and other nuclei (alcohols, phenols, enols, carbodylic acids, amines, amides & mercapto), chemical exchange, effect of deuteration, complex spin-spin interaction between two,three, four and five nuclei (first order spectra), virtual coupling. Stereochemistry, hindered rotation, Karplus curve-variation of coupling constant with dihedral angle. Simplification of complex spectra nuclear magnetic double resonance, contact shift reagents, solvent effects. Fourier transform technique, nuclear Overhauser effect (NOE). Resonance of other nuclei- F, P.

UNIT III

Carbon-13 NMR Spectroscopy

General considerations, chemical shift (Aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbon), coupling constants. Two dimension NMR spectroscopy – COSY, NOESY, DEPT, INEPT, APT and INDEQUATE techniques.

Mass Spectrometry

Introduction, ion production – El, Cl, FD and FAB, factors affecting fragmentation, ion analysis, ion abundance. Mass spectral fragmentation of organic compounds, common functional groups, molecular ion peak, metastable peak, McLafferty rearrangement. Nitrogen

rule. High resolution mass spectrometry. Examples of mass spectral fragmentation of organic compounds with respect to their structure determination.

Books Recommended

1. Textbook of Organic Chemistry 1st Ed., P. S. Kalsi, New Age International (P) Ltd. Pub.
2. Organic Chemistry, R. T. Morrison, & R. N. Boyd, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
3. Organic Spectroscopy, W. Kemp, Palgrave
4. A Complete Introduction to Modern NMR Spectroscopy, Roger S. Macomber, Willey Publication, (1997).
5. Modern NMR Spectroscopy : A Guide for Chemists. J. K. M. Sanders, B. K. Hunter. Oxford UniversityPress, (1993).
6. Principles of nuclear magnetic resonance in one and two dimensions. R. R. Ernst, Geoffrey Bodenhausen, and Alexander Wokaun. Oxford University Press, (1987).
7. Spectrometric Identification of Organic Compounds, R. M. Silverstein, F. X. Webster, D. J. Kiemle, D. L. Bryce, Willey, 8th Ed., (2015).