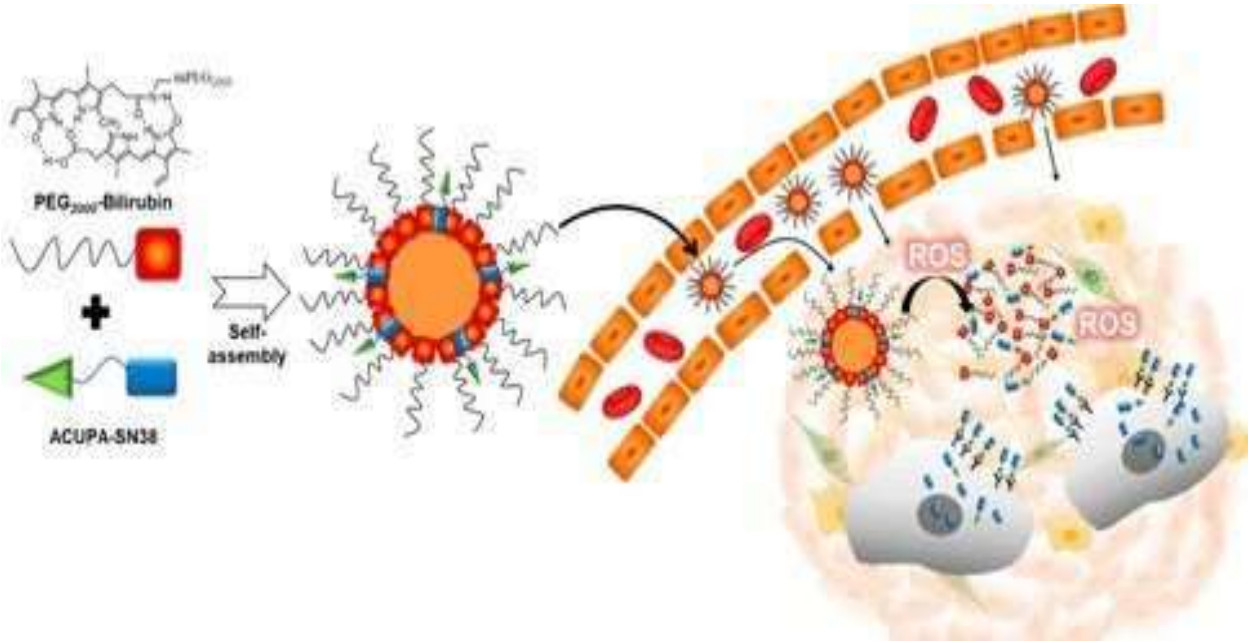
Integrated M.Sc. Chemistry (CBCS)

SYLLABUS



Department of Chemistry
Central University of Tamil Nadu
Thiruvarur 610 005
2018

Programme Structure

Duration	:	10 semesters
Intake	:	30

The five year program is spread into ten semesters where in first four semesters are designed for broad subject based understanding. Later six semesters will have increased focus on chemistry.

The subject courses in the early stage of iM.Sc programme are simplified and of basic level that bolsters the inter-disciplinary way of learning. The third and subsequent year courses have been designed on advanced theories in chemistry with emphasis on concurrent modern laboratory techniques. Further the iM.Sc (Chemistry) programme has been included with experiments that provide exhaustive hands on experience on various sophisticated instruments, experimental techniques to enable the students secure jobs in corporate. The final semester is dedicated to specialization within the subject with research level training.

The rules and regulations of Choice Based Credit System (CBCS) are applicable to this program. Generally, a student takes ten semesters to complete the program. The courses offered under CBCS, has certain credit number (2, 3 or 4). Core requirements of the programs are clearly defined. In the first two years of the program, a student has common course load with students from other departments. From fifth semester onwards, students will have courses more tuned towards chemistry. Apart from courses offered by the Department of Chemistry, student shall take prescribed number of elective courses either from parent department or from other departments.

CENTRAL UNIVERSITY OF TAMIL NADU, THIRUVARUR
iM.Sc. CHEMISTRY SYLLABUS CREDIT DISTRIBUTION

Semester	Title of the Course	Nature of the course	Credit
1	General Chemistry	T	3
1	General Chemistry Laboratory	P	2
1	Second Major	T	3
1	Second Major Laboratory	P	2
1	Third Major	T	3
1	Third Major Laboratory	P	2
1	*****Ability Enhancement Course *****	AECC	2
1	English - 1	AECC	3
2	Physical Chemistry I	T	3
2	Physical Chemistry Laboratory I	P	2
2	Second Major	T	3
2	Second Major Laboratory	P	2
2	Third Major	T	3
2	Third Major Laboratory	P	2
2	*****Ability Enhancement Course *****	AECC	2
2	English – 2	AECC	3
3	Inorganic Chemistry I	T	3
3	Inorganic Chemistry Laboratory I	P	2
3	Second Major	T	3
3	Second Major Laboratory	P	2
3	Third Major	T	3
3	Third Major Laboratory	P	2
3	*****Ability Enhancement Course *****	AECC	2
3	Language - 1	AECC	3
4	Organic Chemistry I	T	3
4	Organic Chemistry Laboratory I	P	2
4	Second Major	T	3
4	Second Major Laboratory	P	2
4	Third Major	T	3
4	Third Major Laboratory	P	2
4	*****Ability Enhancement Course *****	AECC	2
4	Language - 2	AECC	3
5	Analytical Methods in Chemistry	DSE-T	4
5	Acid-bases, redox reactions, s- and p- block elements	DSE-T	4
5	Organic Reaction Mechanisms & Heterocyclic compounds	DSE-T	4
5	Physical States of Matter & Photochemistry	DSE-T	4
5	Analytical & Inorganic Chemistry Laboratory I	DSE-P	2

Semester	Title of the Course	Nature of the course	Credit
5	Organic Chemistry Laboratory II	DSE-P	2
5	Physical Chemistry Laboratory II	DSE-P	2
5	*****Skill Enhancement Course*****	SEC	2
6	Nuclear, Basic Organometallic and Bioinorganic Chemistry	DSE-T	4
6	Reaction Mechanisms and Natural Products Chemistry	DSE-T	4
6	Quantum Chemistry and Molecular Spectroscopy	DSE-T	4
6	Analytical & Inorganic Chemistry Laboratory II	DSE-P	2
6	Organic Chemistry Laboratory III	DSE-P	2
6	Physical Chemistry Laboratory III	DSE-P	2
6	*****Skill Enhancement Course*****	SEC	2
6	*### Project (for students opting exit)**	P	6
7	Solid State, Main Group and Coordination Chemistry	T	4
7	Physical Organic Chemistry & Aromatic Compounds	T	4
7	Chemical Kinetics and Group Theory	T	4
7	*****Subject Selective Elective*****	E	4
7	Advanced Organic Chemistry Laboratory	P	4
8	Advanced Organometallic and Bioinorganic Chemistry	T	4
8	Organic Photochemistry and Rearrangements	T	4
8	Advanced Quantum Mechanics & Molecular Spectroscopy	T	4
8	Physical Methods in Chemistry I	T	4
8	Advanced Physical Chemistry Laboratory	P	4
9	Physical methods in Chemistry II	T	4
9	Molecular Rearrangements and Organic Photochemistry	T	4
9	Thermodynamics (Classical/statistical) & Electrochemistry	T	4
9	*****Subject Selective Elective*****	E	4
9	Advanced Inorganic Chemistry Laboratory	P	4
10	Research Project	P	12

Total: 124 + 6 = 130 credits for B.Sc (Exit) option candidates. Those who opt for exit option should give in writing to the department with an endorsement from the concerned parent at the end of second year (fourth semester).

Total: 196 credits for iMSc Candidates

The I.MSc students with Maths background will be given Maths and Physics as other majors, whereas i.MSc students with Life-Science / Biology background will be given Physics and Life-Science as other major subjects.

Semester I
Title: General Chemistry

Credits: 3 **Theory**

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Course objective:

To introduce the principles and fundamental aspects of chemistry

- Concept of atomic structure & chemical bonding
- Stereochemistry and basic organic chemistry
- Kinetics, equilibrium and Energetics

Course Outcome:

The learners will able to

- know the basic chemistry in a more holistic way
- enthuse the subject
- this course makes them confident and capable of accepting basic science

Atomic Structure:
Review of: Bohr's theory and its limitations, dual behaviour of matter and radiation, de Broglie's relation, Heisenberg Uncertainty principle. Hydrogen atom spectra. Need of a new approach to Atomic structure.

Introduction to Quantum mechanics: Time independent Schrodinger equation and meaning of various terms in it. Significance of ψ and ψ^2, Schrödinger equation for hydrogen atom. Radial and angular parts of the hydogenic wavefunctions (atomic orbitals) and their variations for 1s, 2s, 2p, 3s, 3p and 3d orbitals (Only graphical representation). Radial and angular nodes and their significance. Radial distribution functions and the concept of the most probable distance with special reference to 1s and 2s atomic orbitals. Discovery of spin, spin quantum number (s) and magnetic spin quantum number (m_s). Significance of quantum numbers, orbital angular momentum and quantum numbers m_l and m_s. Shapes of s, p and d atomic orbitals, nodal planes.

Rules for filling electrons in various orbitals, Electronic configurations of the atoms. Stability of half-filled and completely filled orbitals, concept of exchange energy. Relative energies of atomic orbitals, Anomalous electronic configurations.

Chemical Bonding and Molecular Structure:
Ionic Bonding: General characteristics of ionic bonding. Energy considerations in ionic bonding, lattice energy and solvation energy and their importance in the context of stability and solubility of ionic compounds. Statement of Born-Landé equation for calculation of lattice energy, Born-Haber cycle and its applications, polarizing power and polarizability. Fajan's rules, ionic character in covalent compounds, bond moment, dipole moment and percentage ionic character.

Fundamentals of Organic Chemistry:
Physical Effects, Electronic Displacements: Inductive Effect, Electromeric Effect, Resonance and Hyperconjugation. Cleavage of Bonds: Homolysis and Heterolysis. Structure, shape and reactivity of organic molecules: Nucleophiles and electrophiles.

Reactive Intermediates: Carbocations, Carbanions and free radicals. Strength of organic acids and bases: Comparative study with emphasis on factors affecting pK values. Aromaticity: Benzenoids and Hückel's rule.

Organic Stereochemistry:
Conformations with respect to ethane, butane and cyclohexane. Interconversion of Wedge Formula, Newman, Sawhorse and Fischer representations. Concept of chirality (upto two carbon atoms). Configuration: Geometrical and Optical isomerism; Enantiomerism, Diastereomerism and Meso compounds). Threo and erythro; D and L; cis – trans nomenclature; CIP Rules: R/ S (for upto 2 chiral carbon atoms) and E / Z Nomenclature (for upto two C=C systems).

Chemical Energetics:
Review of thermodynamics and the Laws of Thermodynamics. Important principles and definitions of thermochemistry. Concept of standard state and standard enthalpies of formations, integral and differential enthalpies of solution and dilution. Calculation of bond energy, bond dissociation energy and resonance energy from thermochemical data. Variation of enthalpy of a reaction with temperature – Kirchhoff's equation. Statement of Third Law of thermodynamics and calculation of absolute entropies of substances.

Ionic Equilibria:
Strong, moderate and weak electrolytes, degree of ionization, factors affecting degree of ionization, ionization constant and ionic product of water. Ionization of weak acids and bases, pH scale, common ion effect. Salt hydrolysis-calculation of hydrolysis constant, degree of hydrolysis and pH for different salts. Buffer solutions. Solubility and solubility product of sparingly soluble salts – applications of solubility product principle.

Chemical Kinetics:
The concept of reaction rates. Effect of temperature, pressure, catalyst and other factors on reaction rates. Order and molecularity of a reaction. Derivation of integrated rate equations for zero, first and second order reactions (both for equal and unequal concentrations of reactants). Half–life of a reaction. General methods for determination of order of a reaction. Concept of activation energy and its calculation from Arrhenius equation. Theories of Reaction Rates: Collision theory and Activated Complex theory of bimolecular reactions. Comparison of the two theories (qualitative treatment only).

Reference Books

1. R. P. Rastogi, R. R. Misra, An Introduction to Chemical Thermodynamics, 6th edn., Vikas Pub. Pvt. Ltd. **2003.**
2. P. Atkins and J Paula, The elements of Physical chemistry, 7th edn., Oxford University Press
3. K. K. Sharma, L. K. Sharma, A Textbook of Physical Chemistry, 4th edn, Vikas publishing House
4. B. R. Puri, L. R. Sharma, M. S. Pathania, Elements of Physical chemistry, Vishal Pub. Co. Jalandhar
5. G. K. Vemulapalli, Physical Chemistry, Prentice-Hall of India Pvt. Ltd. **(1997).** K. J. Laidler, Chemical kinetics 3rd edn, Pearson education **2004.**

6. Graham Solomons, T. W., Fryhle, C. B., Snyder, S. A., Organic Chemistry, 12th edn, Wiley, **2016.**
7. McMurry, J.E., Fundamentals of Organic Chemistry, 7th edn, Cengage Learning India Edition, **2013.**
8. Sykes, P. A Guidebook to Mechanism in Organic Chemistry, Orient Longman, New Delhi, **1988.**
9. Eliel, E.L. Stereochemistry of Carbon Compounds, Tata McGraw Hill education, **2000.**
10. Finar, I.L. Organic Chemistry (Vol. I & II), Vol I, 6th edn, Pearson Education, **2002**
11. Morrison, R.T., Boyd, R.N. Organic Chemistry, 7th edn, Pearson Education.

Further reading:

1. J. Rajaram and J. C. Kuriakose, Thermodynamics, Shoban Lal Nagin Chand & Co **1986.**
2. H. Kuhn and H. D. Fosterling, Principles of Physical chemistry, John Wiley.
3. W. J. Moore, Basic Physical Chemistry, Orient Longman.
4. F. A. Alberty and R. J. Silby, Physical Chemistry, John Wiley.
5. G. M. Barrow, Physical Chemistry, 5th edn., Tata McGraw Hill.
6. G. W. Castellan, Physical Chemistry, 3rd edn, Narosa Publishing House, New Delhi, **2004.**
7. Clayden,J.,Greeves,N.,Warren.S.Organic Chemistry,2nd edn,Oxford University Press, **2014**

Semester I
General Chemistry Laboratory

Credits: 2 **Practical**

Course objective:

- To measure and estimate the heat transfer of various reactions using calorimeter.
- To measure and understand the importance of p^H in foods and other day to day materials.
- To prepare suitable buffer solutions, check them with their standards and Handle ionic equilibria.

Course outcome:

After successful completion of this course, the students will able

- To understand the techniques/methods to prepare and check buffers.
- To estimate the heats of various reactions.

Thermochemistry:

1. Determination of heat capacity of calorimeter for different volumes.
2. Determination of enthalpy of neutralization of hydrochloric acid with sodium hydroxide.

3. Determination of enthalpy of ionization of acetic acid.
4. Determination of integral enthalpy of solution of salts (KNO3, NH4Cl).
5. Determination of enthalpy of hydration of copper sulphate.
6. Study of the solubility of benzoic acid in water and determination of ΔH.

Ionic Equilibria:

1. Measurement of pH of different solutions like aerated drinks, fruit juices, shampoos and soaps using pH-meter.
2. Preparation of buffer solutions:
    a) Sodium acetate-acetic acid
    b) Ammonium chloride-ammonium hydroxide
3. Measurement of the pH of buffer solutions and comparison of the values with theoretical values.

Reference books

1. B. Viswanathan, Practical Physical chemistry, Viva Pub., **2005**
2. Saroj Kumar and Naba Kumar, Physical Chemistry Practical, New Central Book Agency,**2012**
3. Practical Physical Chemistry Paperback, **1974** by A.M. James, F.E. Prichard.

Semester II
Physical Chemistry I

Credits: 3 **Theory**

Course objective:

- To cover the methods of handling of Chemical Equilibrium, including Le Chatelier's Principle.
- To introduce the concepts of chemistry for handling various ideal and non-ideal solutions.
- To emphasis the Phase Equilibria including congruent and incongruent melting systems.
- A brief introduction on Electrochemistry, Electrochemical Cells and Conductance.

Course outcome:

After successful completion of this course, the students will able

- To control the reactions using Chemical Equilibrium Concepts.
- To handle different types of solution under different C, P, V and T conditions.
- To understand the concepts of different phases and their characteristic properties.
- To understand the batteries, conductance, corrosion etc.

Chemical Equilibrium: Free energy change in a chemical reaction. Thermodynamic derivation of the law of chemical equilibrium. Distinction between ΔG and ΔG_0, Le Chatelier's principle. Relationships between Kp, Kc and Kx for reactions involving ideal gases.

Solutions: Thermodynamics of ideal solutions: Ideal solutions and Raoult's law, deviations from Raoult's law – non-ideal solutions. Vapour pressure-composition and temperature composition curves of ideal and non-ideal solutions. Distillation of solutions. Lever rule. Azeotropes. Partial miscibility of liquids: Critical solution temperature; effect of impurity on partial miscibility of liquids. Immiscibility of liquids- Principle of steam distillation. Nernst distribution law and its applications, solvent extraction.

Phase Equilibrium: Phases, components and degrees of freedom of a system, criteria of phase equilibrium. Gibbs Phase Rule and its thermodynamic derivation. Derivation of Clausius – Clapeyron equation and its importance in phase equilibria. Phase diagrams of one-component systems (water and sulphur) and two component systems involving eutectics, congruent and incongruent melting points (lead-silver, $FeCl_3$-H_2O and Na-K only).

Electrochemistry: Reversible and irreversible cells. Concept of EMF of a cell. Measurement of EMF of a cell. Nernst equation and its importance. Types of electrodes. Standard electrode potential. Electrochemical series. Thermodynamics of a reversible cell, calculation of thermodynamic properties: ΔG, ΔH and ΔS from EMF data. Calculation of equilibrium constant from EMF data. Concentration cells with transference and without transference. Liquid junction potential and salt bridge. pH determination using hydrogen electrode and quinhydrone electrode. Potentiometric titrations -qualitative treatment (acid-base and oxidation-reduction only). Irreversible electrode processes – overvoltage. Corrosion of metals – forms of corrosion, corrosion monitoring and prevention methods.

Conductance: Conductivity, equivalent and molar conductivity and their variation with dilution for weak and strong electrolytes. Kohlrausch law of independent migration of ions. Transference number and its experimental determination using Hittorf and Moving boundary methods. Ionic mobility. Applications of conductance measurements: determination of degree of ionization of weak electrolyte, solubility and solubility products of sparingly soluble salts, ionic product of water, hydrolysis constant of a salt. Conductometric titrations (only acid-base).

Reference Books

1. G.M. Barrow, Physical Chemistry Tata McGraw-Hill **(2007).**
2. Castellan, G.W. Physical Chemistry 4th Ed. Narosa **(2004).**
3. Kotz, J.C., Treichel, P.M. & Townsend, J.R. General Chemistry Cengage Learning India Pvt. Ltd., New Delhi **(2009).**
4. R. P. Rastogi, R. R. Misra, An Introduction to Chemical Thermodynamics, 6th edn., Vikas Pub. Pvt. Ltd. **(2003).**
5. Mahan, B.H. University Chemistry 3rd Ed. Narosa **(1998).** Petrucci, R.H. General Chemistry 5th Ed. Macmillan Publishing Co.: New York **(1985).**
6. B. R. Puri, L. R. Sharma, M. S. Pathania, Elements of Physical chemistry, Vishal Pub. Co. Jalandhar.
7. K. L. Kapoor, A Textbook of Physical Chemistry, Volumes 1, Macmillan India Ltd,
8. P. Atkins and J Paula, The elements of Physical chemistry, 7th edn., Oxford University Press.

Further reading

1. J. Rajaram and J. C. Kuriakose, Thermodynamics, Shoban Lal Nagin Chand & Co **(1986).**
2. H. Kuhn and H. D. Fosterling, Principles of Physical chemistry, John Wiley. W. J. Moore, Basic Physical Chemistry, Orient Longman.
3. D. A. McQuarrie, J. D. Simon, Physical Chemistry – A molecular Approach Viva Books Pvt. Ltd.
4. F. A. Alberty and R. J. Silby, Physical Chemistry, John Wiley.

Semester II
Physical Chemistry Laboratory I

Credits: 2 **Practical**

Course objective

- To construct phase diagram for partially miscible system
- To perform solvent extraction effectively
- To understand the importance of phase diagram and its construction
- To carry out the volumetric titration without indicators and determine the equivalence point.

Course outcome

After successful completion of this course, the students will able

- To estimate and distinguish End point and equivalence point.
- To apply the basic principle of solvent extraction.
- To construct the Phase diagram.

Distribution:

1. Study the partition of solute in two immiscible liquids
2. Study of the equilibrium of the following reactions by the distribution method:

   $I_2(aq) + I^-(aq) \rightarrow I_3^-(aq)$

Phase equilibria:

1. Construction of the phase diagram of a binary system (simple eutectic) using cooling curves.
2. Determination of the critical solution temperature and composition of the phenol water system and study of the effect of impurities on it.

Potentiometry: Perform the following potentiometric titrations:

1. Strong acid vs. strong base
2. Weak acid vs. strong base

Conductance: conductometric titrations:

1. Strong acid vs. strong base
2. Weak acid vs. strong base

Reference Books

1. J.B. Yadav, Advanced Practical Physical Chemistry, Goel Publishing House, **2001.**
2. G.W. Garland, J.W. Nibler, D.P. Shoemaker, Experiments in Physical Chemistry, 8th Edn. McGraw Hill, **2009.**
3. Practical Physical Chemistry Paperback, **1974** by A.M. James, F.E. Prichard.

Semester III
Inorganic Chemistry I

Credit: 3 **Theory**

Objectives

To put forth the ideas of various theories to explain the bonding in inorganic molecules and ions. To introduce the existence of special properties of transition and post transition metals. Introducing the concept of coordination chemistry, nature of ligand, bonding (octahedral and tetrahedral complexes), spectral and magnetic properties.

Learning Outcomes

Gain the knowledge of various bonding theories and ability to predict the existence and non-existence of molecules with special features.

Understanding the reason why the d- and f-block elements exist in various oxidation state, coloured with magnetic and catalytic properties

Perceive in coordination complexes, their bonding, ligand nature make us to wonder how different complexes have different colours and their importance to biological system

Covalent bonding: VB Approach: Shapes of some inorganic molecules and ions on the basis of VSEPR and hybridization with suitable examples of linear, trigonal planar, square planar, tetrahedral, trigonal bipyramidal and octahedral arrangements.
Concept of resonance and resonating structures in various inorganic and organic compounds. MO Approach: Rules for the LCAO method, bonding and antibonding MOs and their characteristics for s-s, s-p and p-p combinations of atomic orbitals, nonbonding combination of orbitals, MO treatment of homonuclear diatomic molecules of 1^{st} and 2^{nd} periods (including idea of s-p mixing) and heteronuclear diatomic molecules such as HF, CO, NO and NO^+. Polyatomic molecules BeH_2, BH_3 and NH_3 - Walsh diagram. Comparison of VB and MO approaches.

Transition Elements (3d series): General group trends with special reference to electronic configuration, variable valency, colour, magnetic and catalytic properties, ability to form complexes and stability of various oxidation states (Latimer diagrams) for Mn, Fe and Cu.

Lanthanoids and actinoids: Electronic configurations, oxidation states, colour, magnetic properties, lanthanide contraction, separation of lanthanides (ion exchange method only).

Coordination Chemistry-I: ligands, IUPAC nomenclature – coordination number, geometries and isomerism. Theories of coordination compounds - Werner's theory

Valence Bond Theory (VBT): Inner and outer orbital complexes of Cr, Fe, Co, Ni and Cu (coordination numbers 4 and 6). Structural and stereoisomerism in complexes with coordination numbers 4 and 6. Drawbacks of VBT.

Crystal Field Theory: Crystal field effect, octahedral symmetry. Crystal field stabilization energy (CFSE), Crystal field effects for weak and strong fields. Tetrahedral symmetry. Factors affecting the magnitude of 10Dq. Spectrochemical series. Comparison of CFSE for O_h and T_d complexes, spectral and magnetic properties, application of CFT, Tetragonal distortion of octahedral geometry. Jahn-Teller distortion, Square planar coordination.

Reference Books

1. Mahan, B.H. University Chemistry 3rd Ed. Narosa **1998.**
2. Petrucci, R.H. General Chemistry 5th Ed. Macmillan Publishing Co.: New York **1985.**
3. Cotton, F.A. & Wilkinson, G. Basic Inorganic Chemistry, Wiley.
4. Shriver, D. Atkins, P. W.; Inorganic Chemistry, W. H. freeman and Company,5th edition, **2009.**
5. Wulfsberg, G. Inorganic Chemistry, Viva Books Pvt. Ltd. **2014.**
6. Lee, J.D. Concise Inorganic Chemistry ELBS, **1991**.
7. Douglas, B.E., McDaniel, D.H. & Alexander, J.J. Concepts and Models in Inorganic Chemistry, John Wiley & Sons. **2010.**
8. Huheey, J.E., Keiter, E.A., Keiter, R.L. & Medhi, O.K. Inorganic Chemistry: Principles of Structure and Reactivity, Pearson Education India, **2006.**
9. Rao, C. N. R. Understanding Chemistry, University Press (India) Ltd., **2001.**
10. R.P. Sarkar, General and Inorganic Chemistry Part- I, 3rd revised edition; New Central Book Agency, **2011**.

Semester III
Inorganic Chemistry Laboratory I

Credit: 2 **Practical**

Objectives

To introduce the basic analytical technique qualitative and quantitative analysis for mixture of substance with the help of acid- base theory, common ion effect, solubility product, ionic product concepts

Learning Outcomes

Ability to identify the mixture of ions through semi micro qualitative analysis and estimation of various ions through different titrimetric methods

Volumetric Analysis:

1. Estimation of sodium carbonate and sodium hydrogen carbonate present in a mixture.
2. Estimation of oxalic acid by titrating it with $KMnO_4$.
3. Estimation of water of crystallization in Mohr's salt by titrating with $KMnO_4$.
4. Estimation of Fe (II) ions by titrating it with $K_2Cr_2O_7$ using internal indicator.
5. Estimation of Cu (II) ions iodometrically using $Na_2S_2O_3$.
6. Estimation of (i) Mg^{2+} or (ii) Zn^{2+} by complexometric titrations using EDTA.

7. Estimation of total hardness of a given sample of water by complexometric titration.

Qualitative Analysis:

Semi-micro qualitative analysis using H_2S of mixtures - not more than four ionic species (two anions and two cations and excluding insoluble salts) out of the following:

Cations : NH_4^+, Pb^{2+}, Ag^+, Bi^{3+}, Cu^{2+}, Cd^{2+}, Sn^{2+}, Fe^{3+}, Al^{3+}, Co^{2+}, Cr^{3+}, Ni^{2+}, Mn^{2+}, Zn^{2+}, Ba^{2+}, Sr^{2+}, Ca^{2+}, K^+
Anions : CO_3^{2-} , S^{2-}, SO_2^-, $S_2O_3^{2-}$, NO_3^-, CH_3COO^-, Cl^-, Br^-, I^-, NO_3^-,SO_4^{2-}, PO_4^{3-}, BO_3^{3-} ,$C_2O_4^{2-}$, F^- (Spot tests should be carried out wherever feasible)

Reference Books

1. In-house manual prepared by Department of Chemistry, CUTN, Thiruvarur.
2. Svehla, G. Vogel's Qualitative Inorganic Analysis, Pearson Education, **2012.** Mendham, J. Vogel's Quantitative Chemical Analysis, Pearson, **2009.**
3. Jeffery, G. H., Bassett, J., Mendham, J., Denney, and R. C., Vogel's quantitative chemical analysis, 5th edition, Longman Scientific and Technical, **1989.**
4. Mendham, J., Denney, J. C., Barnes, J. D., and Thomas, M. J. K., : Vogel's Prescribed book of qualitative chemical analysis, 6th Edition, Prentice Hall, **2000.**
5. Morris Hein, Judith N. Peisen and Robert L. Miner, Foundations of College
6. Chemistry in the Laboratory, John Wiley and Sons, **2011.**
7. Woollins, J. D; Inorganic experiments, 3rd Edition, Wiley-VCH Verlag GmbH Co.**2012.**
8. Ghoshal, Mahapatra and Nad, An Advanced Course in Practical Chemistry, New Central Book Agency, **2011**.

Semester IV
Organic Chemistry I

Credits: 3 **Theory**

Specific objectives:
Preparation concepts and the properties of different types of organic molecules and functional groups.

Learning outcomes:
Ensures students to understand and acquire knowledge on preparation and the properties of different types of organic molecules and functional groups.

Functional group approach for the following reactions (preparations & reactions) to be studied in context to their structure.

Aromatic hydrocarbons: Preparation (case benzene) from phenol, by decarboxylation, from acetylene, from benzene sulphonic acid. Reactions: (case benzene): Electrophilic substitution: nitration, halogenation and sulphonation. Friedel-Craft's reaction (alkylation and acylation) (upto 4 carbons on benzene). Side chain oxidation of alkyl benzenes (upto 4 carbons on benzene).

Alkyl and Aryl Halides, Aryalkyl Halides (Upto 5 carbons): Types of Nucleophilic Substitution (S_N1, S_N2 and S_Ni) reactions. Preparation: from alkenes and alcohols. Reactions: hydrolysis, nitrite & nitro formation, nitrile & isonitrile formation. Williamson's ether synthesis: Elimination vs substitution. Aryl Halides Preparation: (Chloro, bromo and iodo-benzene case): from phenol, Sandmeyer & Gattermann reactions. Reactions (Chlorobenzene): Aromatic nucleophilic substitution (replacement by –OH group) and effect of nitro substituent. Benzyne Mechanism: KNH_2/NH_3 (or $NaNH_2/NH_3$). Reactivity and Relative strength of C-Halogen bond in alkyl, allyl, benzyl, vinyl and aryl halides.

Alcohols, Phenols and Ethers (Upto 5 Carbons): Alcohols: Preparation of 1°, 2° and 3° alcohols: using Grignard reagent, Ester hydrolysis, Reduction of aldehydes, ketones, carboxylic acid and esters. Reactions: With sodium, HX (Lucas test), esterification, oxidation (with PCC, alk. $KMnO_4$, acidic dichromate, conc. HNO_3). Oppeneauer oxidation Diols: (Upto 6 Carbons) oxidation of diols.

Phenols: Preparation: Cumene hydroperoxide method, from diazonium salts. Reactions: Electrophilic substitution: Nitration, halogenation and sulphonation. Reimer Tiemann reaction, Gattermann-Koch reaction, Houben–Hoesch Condensation, Schotten – Baumann Reaction. Ethers (aliphatic and aromatic): Cleavage of ethers with HI.

Aldehydes and ketones (aliphatic and aromatic): (Formaldehye, acetaldehyde, acetone and benzaldehyde) Preparation: from acid chlorides and from nitriles. Reactions – Reaction with HCN, ROH, $NaHSO_3$, NH_2-G derivatives. Iodoform test. Aldol Condensation, Cannizzaro's reaction, Wittig reaction, Benzoin condensation. Clemensen reduction and Wolff Kishner reduction. Meerwein-Pondorff Verley reduction.

Carboxylic acids and their derivatives Carboxylic acids (aliphatic and aromatic): Preparation: Acidic and Alkaline hydrolysis of esters. Reactions: Hell – Vohlard - Zelinsky Reaction. Carboxylic acid derivatives (aliphatic): (Upto 5 carbons) Preparation: Acid chlorides, Anhydrides, Esters and Amides from acids and their interconversion. Reactions: Comparative study of nucleophilicity of acyl derivatives. Reformatsky Reaction, Perkin condensation.

Amines and Diazonium Salts Amines (Aliphatic and Aromatic) (Upto 5 carbons): Preparation: from alkyl halides, Gabriel's Phthalimide synthesis, Hofmann Bromamide reaction. Reactions: Hofmann vs. Saytzeff elimination, Carbylamine test, Hinsberg test, with HNO_2, Schotten – Baumann Reaction. Electrophilic substitution (case aniline): nitration, bromination, sulphonation. Diazonium salts: Preparation: from aromatic amines. Reactions: conversion to benzene, phenol, dyes.

Amino Acids, Peptides and Proteins: Preparation of Amino Acids: Strecker synthesis using Gabriel's phthalimide synthesis. Zwitterion, Isoelectric point and Electrophoresis. Reactions of Amino acids: ester of –COOH group, acetylation of $–NH_2$ group, complexation with Cu^{2+} ions, ninhydrin test. Overview of Primary, Secondary, Tertiary and Quaternary Structure of proteins. Determination of Primary structure of Peptides by degradation Edmann degradation (N-terminal) and C–terminal (thiohydantoin and with carboxypeptidase enzyme). Synthesis of simple peptides (upto dipeptides) by N-protection (t-butyloxycarbonyl and phthaloyl) and carbon activating groups and Merrifield solid-phase synthesis.

Carbohydrates: Classification, and General Properties, Glucose and Fructose (open chain and cyclic structure), Determination of configuration of monosaccharides, absolute configuration of Glucose and Fructose, Mutarotation, ascending and descending in monosaccharides. Structure of disacharrides (sucrose, cellobiose, maltose, lactose) and polysacharrides (starch and cellulose) excluding their structure elucidation.

Reference Books

1. Barrow, G.M. Physical Chemistry Tata McGraw-Hill **(2007).**
2. Castellan, G.W. Physical Chemistry 4th Ed. Narosa **(2004).**
3. Kotz, J.C., Treichel, P.M. & Townsend, J.R. General Chemistry, Cengage Learning India Pvt. Ltd.: New Delhi **(2009).**
4. Mahan, B.H. University Chemistry, 3rd Ed. Narosa **(1998).**
5. Petrucci, R.H. General Chemistry, 5th Ed., Macmillan Publishing Co.: New York **(1985).**
6. Finar, I.L. Organic Chemistry, Vol I, 6th edn, Pearson Education, **2002.**
7. Finar, I.L. Organic Chemistry, Vol II, 5th edn, Pearson Education India, **2002.**
8. Morrison, R.T., Boyd, R.N. Organic Chemistry, 7th edn, Pearson Education, **2010.**
9. Nelson, D. L., Cox, M. M. Lehninger, Principles of Biochemistry, 7th edn., WH Freeman, **2017.**
10. Berg, J.M., Tymoczko, J.L., Stryer, L. Biochemistry, 5th edn, W.H.Freeman and Co Ltd, **2002.**

Semester IV
Organic Chemistry Laboratory I

Credits: 2 **Practical**

Specific objectives:

To introduce the basic concepts of organic chemistry such as separation, purification techniques and qualitative analysis of organic compounds through simple experiments.

Learning outcomes:

Students will gain hands-on experience to an introductory level synthetic organic chemistry lab, through the experiments involving purification techniques, identification of functional groups and separation of simple organic compounds.

1. **Organic Qualitative Analysis:** Systematic Qualitative Analysis of Organic Compounds possessing monofunctional groups (-COOH, phenolic, aldehydic, ketonic, amide, nitro, amines) and preparation of one derivative.

2. Preparations and characterizations:

Separation of amino acids/organic compounds by chromatography (paper/TLC).

a. Titration curve of glycine.
b. Action of salivary amylase on starch and effect of temperature
c. Differentiation between a reducing and a nonreducing sugar.

Reference Books

1. Vogel, A.I., Tatchell, A.R., Furnis, B.S., Hannaford, A.J. & Smith, P.W.G., Textbook of Practical Organic Chemistry, Prentice-Hall, 5th edition, **1996**
2. Mann, F.G. & Saunders, B.C. Practical Organic Chemistry Orient-Longman, **1960.**
3. Ahluwalia, V.K. & Aggarwal, R. Comprehensive Practical Organic Chemistry, Universities Press.

Semester V
Analytical Methods in Chemistry

Credit: 4 **Theory**

Course objective

- Significant and elementary of mathematical and statistical data, errors, and test.
- Systematic performance of qualitative and quantitative remarks in analytical methods.
- Essential law of spectroscopy with their specific rules and validity.
- Consistency between scientific, technical, limitations and analytical information.

Course outcome

After successful completion of this course, the students will able

- To develop the analytical view in qualitative and quantitative analysis
- To know Spectrometers are used to identify the molecules as per their transition, rotational, vibrational, translation motion of the molecules.
- To understand Methodology of separation techniques, and their essential contents during the removal of wastages

Qualitative and quantitative aspects of analysis: Sampling, evaluation of analytical data, errors, accuracy and precision, methods of their expression, normal law of distribution if indeterminate errors, statistical test of data; F, Q and t test, rejection of data, and confidence intervals.

Optical methods of analysis: Origin of spectra, interaction of radiation with matter, fundamental laws of spectroscopy and selection rules, validity of Beer-Lambert's law.
UV-Visible Spectrometry: Basic principles of instrumentation (choice of source, monochromator and detector) for single and double beam instrument; **Basic principles of quantitative analysis:** estimation of metal ions from aqueous solution, geometrical isomers, keto-enol tautomers. Woodward–Fieser Rules, Determination of composition of metal complexes using Job's method of continuous variation and mole ratio method.
Infrared Spectrometry: Basic principles of instrumentation (choice of source, monochromator & detector) for single and double beam instrument; sampling techniques. Structural illustration through interpretation of data, Effect and importance of isotope substitution.
Flame Atomic Absorption and Emission Spectrometry: Basic principles of instrumentation (choice of source, monochromator, detector, choice of flame and Burner designs. Techniques of atomization and sample introduction; Method of background

correction, sources of chemical interferences and their method of removal. Techniques for the quantitative estimation of trace level of metal ions from water samples.

Thermal methods of analysis: Theory of thermogravimetry (TG), basic principle of instrumentation. Techniques for quantitative estimation of Ca and Mg from their mixture.

Electroanalytical methods: Classification of electroanalytical methods, basic principle of pH metric, potentiometric and conductometric titrations. Techniques used for the determination of equivalence points. Techniques used for the determination of pKa values.

Separation techniques: Solvent extraction: Classification, principle and efficiency of the technique. Mechanism of extraction: extraction by solvation and chelation. Technique of extraction: batch, continuous and counter current extractions. Qualitative and quantitative aspects of solvent extraction: extraction of metal ions from aqueous solution, extraction of organic species from the aqueous and nonaqueous media. Chromatography: Classification, principle and efficiency of the technique. Mechanism of separation: adsorption, partition & ion exchange. Development of chromatograms: frontal, elution and displacement methods. Qualitative and quantitative aspects of chromatographic methods of analysis: IC, GLC, GPC, TLC and HPLC.

Reference Books

1. Jeffery, G.H., Bassett, J., Mendham, J. & Denney, R.C. Vogel's Textbook of Quantitative Chemical Analysis, John Wiley & Sons, **1989.**
2. Willard, H.H., Merritt, L.L., Dean, J. & Settoe, F.A. Instrumental Methods of Analysis, 7th Ed. Wadsworth Publishing Company Ltd., Belmont, California, USA, **1988.**
3. Christian, G.D; Analytical Chemistry, 6th Ed. John Wiley & Sons, New York, **2004.**
4. Harris, D. C. Exploring Chemical Analysis, Ed. New York, W.H. Freeman, **2001.**
5. Khopkar, S.M. Basic Concepts of Analytical Chemistry. New Age, International Publisher, **2009.**
6. Skoog, D.A. Holler F.J. & Nieman, T.A. Principles of Instrumental Analysis, Cengage Learning India Ed.
7. Mikes, O. Laboratory Hand Book of Chromatographic & Allied Methods, Elles Harwood Series on Analytical Chemistry, John Wiley & Sons, **1979.**
8. Ditts, R.V. Analytical Chemistry; Methods of Separation, van Nostrand, **1974.**

Semester V

Acid-bases, Redox Reactions, s- and p- block Elements

Credit: 4 **Theory**

Objectives:

To introduce the concept of acid-bases and their behaviours in different solvent systems, principles of redox reactions, knowledge of s and p- block elements and their compounds.

Learning Outcomes:

Ensures the students to gain the concept of acids and bases in different solvents, knowledge of oxidation and reduction reactions, oxidation numbers and relevant diagrams in relation to ore extractions. Basic properties and uses of s- and p-block elements and their compounds.

Acids and Bases, Chemistry of Aqueous and Non-aqueous Solvents: Theory of Acid bases: Bronsted-Lowry theory, Lewis theory, Lux-Flood definition, Usanovich definition, HSAB theory and symbiosis - Gas phase acid-base chemistry – Solvent levelling effects. Chemistry in aqueous and Non-aqueous Solvents - super acids - molten salts.

Oxidation and Reduction Reactions: Oxidation and reduction reactions – oxidation number concept, balancing redox equations by oxidation number method and ion-electron method – equivalent weight of oxidizing and reducing agents. Disproportionation and comproportionating reaction, Redox stability in water: Frost-Ebsworth, Latimer and Pourbaix diagrams, applications of redox reactions to extraction of elements from their ores Ellingham diagrams

s- and p-Block Elements: Recapitulation of s-block elements.

Boron Group: Introduction; oxidation states, hydrides, halides, oxides, oxo acids, hydroxides, oxoanions, nitrogen and phosphorous derivatives. Al, Ga, In and Tl salts of oxoacids and aqueous solution chemistry, organometallic compounds.

Carbon Group: Introduction; allotropes of carbon, Intercalation compounds of graphite; hydrides, carbides, silicides, halides, oxides, oxo acids, hydroxides; silicates; silicones, cyanogen, its derivatives and silicon nitride; aqueous solution chemistry and oxoacid salts of Sn and Pb.

Nitrogen Group: Introduction; oxidation states, hydrides; halides; oxides; oxo acids; salts of oxo acids; oxo anions; hydroxides; nitrides, phosphides and arsenides; Phosphazenes; aqueous solution chemistry; organic derivatives.

Oxygen Group and Halogen Family: Oxygen group: Introduction – Hydrides; Halides, Oxohalides and complex halides – Oxides, Oxoacids and their salts – Sulphur-nitrogen compounds – Aqueous solution chemistry of S, Se and Te – Organic derivatives.
Halogen family: comparative study of halogens and their compounds – Oxides and oxoacids of halogens (structure only) – Basic properties of halogens – Inter-halogen compounds – preparation, properties and uses – Pseudohalogens – Preparation, properties and uses of cyanogens and thiocyanogen comparison with halogens – Anomalous properties of fluorine.

Noble gases: Introduction – compounds of Xe, Kr and Rn – Preparation, structure and bonding – Reactivity

Prescribed Books

1. Huheey J. E., Keiter E. A. and Keiter R. L. and Medhi O. K., Inorganic Chemistry - Principles of Structure and Reactivity, 4th edition, Pearson Education, **2006**.
2. Atkins P., Overton T., Rourke J., Weller M. and Armstrong F., Inorganic Chemistry, 5th edition, Oxford University Press, **2010**
3. Lee J. D., Concise Inorganic Chemistry, 5th Eeition, Blackwell Science, **1996**.
4. Miessler G. L. and Tarr D. A., Inorganic Chemistry, 3rd edition, Pearson, **2004**.

Reference Books

1. E. Stocchi: Industrial Chemistry, Vol-I, Ellis Horwood Ltd. UK.
2. R. M. Felder, R. W. Rousseau: Elementary Principles of Chemical Processes, Wiley Publishers, New Delhi.
3. Greenwood, N. N., and Earnshaw, A., Chemistry of the Elements, 2nd edition, Elsevier, **2005.**
4. Housecraft, C. E. and Sharpe, A. G., Inorganic Chemistry, 4th edition, Pearson, **2012.**
5. Massey, A. G., Main Group Chemistry, 2nd edition, John and Wiley & Sons, LTD, **2000.**
6. Cotton, F. A., Wilkinson, G., Murillo, C. A. and Bochmann, M.; Advanced Inorganic Chemistry, 6th Edition, John Wiley & Sons, **2008.**
7. Douglas, B., McDaniel, D. and Alexander, J., Concepts and Models of Inorganic Chemistry, 3rd Edition, John Wiley & Sons, **2010**.

Semester V
Organic Reaction Mechanisms and Heterocyclic Compounds

Credit: 4 **Theory**

Specific objectives:

To introduce the concepts of organic reaction mechanisms and preparation, properties of heterocyclic compounds.

Learning outcomes:

Ensures the students to understand and acquire knowledge on the basics of organic reaction mechanisms, synthetic transformations and heterocyclic compounds.

Nucleophilic Substitution: Structural and Solvation Effects on Reactivity: Characteristics of Nucleophilicity; Effect of Solvation on Nucleophilicity; Leaving-Group Effects ; Steric and Strain Effects on Substitution and Ionization Rates ; Effects of Conjugation on Reactivity; Neighboring-Group Participation Structure and Reactions of Carbocation Intermediates; Structure and Stability of Carbocations; Direct Observation of Carbocations;

Competing Reactions of Carbocations; Mechanisms of Rearrangement of Carbocations ;Bridged (Nonclassical) Carbocations.

Polar Addition and Elimination Reactions: Sulfenylation and Selenenylation: Addition Reactions Involving Epoxides; Epoxides from Alkenes and Peroxidic Reagents Subsequent Transformations of Epoxides; Electrophilic Additions Involving Metal Ions; Solvomercuration
Argentation—the Formation of Silver Complexes;Synthesis and Reactions of Alkylboranes Hydroboration; Reactions of Organoboranes;Enantioselective Hydroboration ;Comparison of Electrophilic Addition Reactions ;Additions to Alkynes and Allenes;Hydrohalogenation and Hydration of Alkynes ;Halogenation of Alkynes; Mercuration of Alkynes; Overview of Alkyne Additions ; Additions to Allenes.; E1, E2, E1cb and pyrolytic eliminations.

Carbanion and other nucleophiles: Acidity of hydrocarbons – carbanion character of organometallic compounds – carbanions stabilized by functional groups – enols, enamines and imines – carbanions as nucleophiles in S_N2 reactions.

Heterocyclic compounds: Five membered rings, structure and source of pyrrole, furan, thiophene; Electrophilic substitution of pyrrole, furan, thiophene; reactivity and orientation; saturated five membered heterocycles; six membered rings; structure and source of pyridine compounds; Electrophilic substitution of pyridine and nucleophilic substitution of pyridine; basicity of pyridine and reduction of pyridine.

Prescribed Books

1. Carey, F.A., Sundberg, R.J., Advanced Organic Chemistry, Part A: Structure and Mechanisms, 5th edn, Springer, **2007.**
2. Carey, F.A., Sundberg, R.J., Advanced Organic Chemistry, Part B: Reaction and Synthesis, 5th edn, Springer, **2007.**

Reference Books

1. Finar, I.L. Organic Chemistry, Vol I, 6th edn, Pearson Education, **2002**
2. Finar, I.L. Organic Chemistry, Vol II, 5th edn, Pearson Education India, **2002**
3. Morrison, R.T., Boyd, R.N. Organic Chemistry, 7th edn, Pearson Education, **2010.**
4. Pine, S. H., Organic Chemistry, 5th edn, Tata McGraw Hill Education, **2006.**
5. Smith M. B.,March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 7th edn, Wiley, **2015.**
6. Clayden,J.,Greeves,N.,Warren.S.Organic Chemistry,2nd edn,Oxford University Press, **2014**
7. Sykes, P. A Guidebook to Mechanism in Organic Chemistry, 6th edn, Pearson Education, **2003.**
8. Joule, J.A., Mills, K, Heterocylic Chemistry, 5th edn, Wiley-Blackwell, **2010.**
9. Katritzky, A, R., Ramsden, C. A., Joule, J. A., Zhdankin, V. V., Handbook of Heterocyclic Chemistry 3rd edn, Elsevier, **2010.**
10. Bansal, R. K., Heterocyclic Chemistry, 5th edn, New Age International Private Limited, **2017**

Semester V

Physical States of Matter & Photochemistry

Credits: 4 **Theory**

Course objective:

- To get an overview of Physical states of matter and photochemistry.
- To familiarize about the Kinetic theory of gasses and critical phenomenon
- To introduce the Molecular interactions in liquid and types of liquid crystals.
- To understand the basics of group theory and symmetry
- To get an overview of Photochemistry

Course outcome:

After completion of this course, the students will able to

- To apply various techniques for determine the structure of physical states of matter
- To understand the symmetry of molecules.
- To apply spectrometric techniques to identify the molecules as per their transition, rotational, vibrational and translation motion.

Gaseous State:

Postulates of Kinetic Theory of Gases and derivation of the kinetic gas equation. Maxwell Boltzmann distribution laws of molecular velocities and molecular energies (graphic representation – derivation not required) and their importance. Collision diameter, mean free path, Viscosity of gases and effect of temperature and pressure on coefficient of viscosity (qualitative treatment only).

Real gases: compressibility factor z, van der Waals equation of state – derivation and application in explaining real gas behaviour. Andrews isotherms of CO_2. Deviation of real gases from ideal behaviour, compressibility factor, causes of deviation. Van der Waals equation of state for real gases. van der Waals equation expressed in virial form – calculation of Boyle temperature, Isotherms of real gases, continuity of states. Critical phenomena, critical constants and their calculation from van der Waals equation. Virial. Liquefaction of gases (based on Joule-Thomson effect).

Liquid State:

Intermolecular forces in liquids (qualitative idea only), Structure of liquids. Unusual behavior of water. Surface tension of liquids, surface tension and temperature, interfacial tension, surface active agents, the Parachor and chemical constitution (atomic and structural parachor), Surface tension and its determination using stalagmometer. Viscosity of a liquid and determination of coefficient of viscosity using Ostwald viscometer. Effect of temperature on surface tension and coefficient of viscosity of a liquid (qualitative treatment only).

Liquid Crystals:

Liquid crystals thermographic behaviour. Classification, structure of nematic and cholestric phases. Applications of liquid crystals.

Symmetry:
Symmetry of molecules-symmetry elements and symmetry operations – centre of symmetry, plane of symmetry, proper and improper axes of symmetry, combination of symmetry elements, Group multiplication table, Schoenflies symbols, Determination of point groups of simple molecules like H_2O, NH_3 and BF_3, crystallographic point groups symmetry.

Solid State:
Forms of solids. unit cells, crystal systems, Bravais lattice types and identification of lattice planes. Laws of Crystallography - Law of constancy of interfacial angles, Law of rational indices. Miller indices. X–Ray diffraction by crystals, Bragg's law. Structures of NaCl, KCl and CsCl (qualitative treatment only). Defects in crystals. Glass-Supercooled liquid.

Photochemistry:
Laws of photochemistry-Grothus-Draper law, Stark-Einstein law. Jablonsky diagram qualitative description of fluorescence, phosphorescence, non-radiative processes (internal conversion, intersystem crossing). Quenching of fluorescence. Quantum yield, examples of low and high quantum yields, photochemical reactions (decomposition of HBr, isomerisation of maleic acid to fumaric acid), photosensitised reactions (photosynthesis, isomerization of 2-butene), chemiluminescence, bioluminescence.

Reference books

1. K. L. Kapoor, A Textbook of Physical chemistry, Volumes 1, Macmillan India Ltd
2. B. R. Puri, L. R. Sharma, M. S. Pathania, Elements of Physical chemistry, Vishal Pub. Co.
3. P. Atkins and J. Paula, The elements of Physical chemistry, 7th edn., Oxford University Press
4. D. A. McQuarrie, J. D. Simon, Physical Chemistry – A molecular Approach, Viva Books Pvt. Ltd
5. K. J. Laidler and J. M. Meiser, Physical Chemistry 3rd Edition, Houghton Mifflin Comp., New York, International Edition, **1999.**
6. K. K. Sharma, L R Sharma, A textbook of Physical Chemistry, Vikas Publishing house
7. I. N. Levine, Physical Chemistry, Tata Mc Graw Hill
8. Gurdeep Raj, Photochemistry, 6th Edn, Goel Publishing House, **2014**
9. Rohatgi-Mukherjee, Fundamentals of Photochemistry, New Age International (P) Ltd.
10. V. Ramakrishnan and M. S. Gopinathan: Group Theory in chemistry, Vishal Publication, **1986.**

Further reading

1. J. Rajaram and J. C. Kuriakose, Thermodynamics, Shoban Lal Nagin Chand & Co **1986.**
2. H. Kuhn and H. D. Fosterling, Principles of Physical chemistry, John Wiley.
3. W. J. Moore, Basic Physical Chemistry, Orient Longman.
4. H. Kuhn and H. D. Fosterling, Principles of Physical chemistry, John Wiley.

5. F. A. Alberty and R. J. Silby, Physical Chemistry, John Wiley.
6. G. M. Barrow, Physical Chemistry, 5th edn., Tata McGraw Hill.
7. G. W. Castellan, Physical Chemistry, 3rd edn, Narosa Publishing House, New Delhi, **2004.**
8. N. J. Turro, Modern Molecular Photochemistry, 4th Edition University Science Books, Sausalito, **1991.**
9. F. A. Cotton: Chemical Applications of Group Theory, Wiley Eastern, **1985**.
10. D. M. Bishop, Group theory and Chemistry, Dover, **1989.**

Semester V
Analytical & Inorganic Chemistry Laboratory I

Credit: 2 **Practical**

Objectives:

To introduce the hands on experience on quantitative separation and estimation of metal ions from a mixture. To determine the composition and concentration of a compound in solution with spectroscopic method.

Learning Outcomes:

Students will be able to estimate different metal ions present in a mixture by volumetrically and gravimetrically. They will gather experience on handling UV-Vis spectroscopy for determination of concentration of a compound in solution.

1. Estimation of inorganic compound in a mixture by Volumetric and Gravimetric analysis. A mixture of solution(s) should be given for estimation

1. Cu (V) and Ni (G)
2. Fe (V) and Zn (G)
3. Fe (V) and Ni (G)
4. Zn (V) and Cu (G)

2. Draw calibration curve (absorbance at λ_{max} vs. concentration) for various concentrations of a given coloured compound ($KMnO_4$/ $CuSO_4$) and estimate the concentration of the same in a given solution.
3. Determine the composition of the Fe^{3+}-salicylic acid complex solution by Job's method.

Reference Books

1. Svehla, G. Vogel's Qualitative Inorganic Analysis, Pearson Education, **2012.** Mendham, J. Vogel's Quantitative Chemical Analysis, Pearson, **2009.**
2. In-house manual prepared by Department of Chemistry, CUTN, Thiruvarur.
3. Ghoshal, Mahapatra and Nad, An Advanced Course in Practical Chemistry, New Central Book Agency, **2011.**
4. Venkateswaran V. Veerasamy R. Kulandaivelu A.R., Basic principles of Practical Chemistry, 2nd edition, New Delhi, Sultan Chand & sons, **1997.**
5. M. Hein, J. N. Peisen and R. L.Miner, Foundations of College Chemistry in the Laboratory, John Wiley and Sons, **2011.**

Semester V

Organic Chemistry Laboratory II

Credit: 2 **Practical**

Specific objectives:

To introduce the experimental aspects of organic chemistry involving one step synthesis, separation and qualitative analysis of organic compounds.

Learning outcomes:

Students will gain hands-on experience in one step synthesis, separation and qualitative analysis of organic compounds

1. Qualitative characterization of organic compounds and detection of extra elements (N, S, Cl, Br, I) in organic compounds

2. Identification and separation of a given mixture of organic compounds (organic compounds/amino acids such as glycine, aspartic acid, glutamic acid, tyrosine or any other amino acid).

3. Preparations, purifications of organic compounds (eg.) and discussions on mechanisms

(a) Bromination of phenol/aniline
(b) Benzoylation of amines/phenols
(c) Oxime and 2,4-dinitrophenylhydrazone of aldehyde/ketone
(d) Diazotization of arylamines

Reference Books

1. Vogel, A.I., Tatchell, A.R., Furnis, B.S., Hannaford, A.J., Smith, P.W.G., Textbook of Practical Organic Chemistry, Prentice-Hall, 5th edn**, 1996.**
2. Mann, F.G., Saunders, B.C. Practical Organic Chemistry, 4th edn, Pearson Education India, **2009**
3. Khosla, B. D.; Garg, V. C. & Gulati, A. Senior Practical Physical Chemistry, R. Chand & Co.: New Delhi, **2011.**
4. Qualitative Organic Analysis, Quantitative Organic Analysis, Pearson Education, **2011.**
5. Leonard, J., Lygo, B., Procter. G., Advanced Practical Organic Chemistry, 3rd edn, CRC Press, **2013.**
6. Cranwell, P. B., Harwood, L. M., Moody, C. J., Experimental Organic Chemistry, 3rd edn, Wiley-Blackwell, **2017.**
7. Ahluwalia, V.K., Aggarwal, R. Comprehensive Practical Organic Chemistry, Universities Press, **2004**

Semester V

Physical Chemistry Laboratory II

Credit: 2 **Practical**

Course objective:

- To use the minor lab equipment like Ostwald viscometer, Stalagmometer etc
- To optimize the instrument parameters especially conductivity cell.
- To understand the factors affecting rate of reaction.
- To determine the molecular weight and molecular aggregation.

Course outcome:

After successful completion of this course, the student will able

- To estimate the composition of solutions by measuring the physical parameter.
- To get an idea about the influence of acid strength/type on reaction rate.
- To get a hands-on experience of titrimetric estimation of colored solutions

Surface tension measurement (use of organic solvents excluded)

a) Determination of the surface tension of a liquid or a dilute solution using a stalagmometer.

b) Study of the variation of surface tension of a detergent solution with concentration.

Viscosity measurement (use of organic solvents excluded).

a) Determination of the relative and absolute viscosity of a liquid or dilute solution using an Ostwald's viscometer.

b) Study of the variation of viscosity of an aqueous solution with concentration of solute.

Chemical Kinetics

a) Initial rate method: Iodide-persulphate reaction

b) Integrated rate method:

i. Acid hydrolysis of methyl acetate with hydrochloric acid.

ii. Saponification of ethyl acetate.

iii. Compare the strengths of HCl and H_2SO_4 by studying kinetics of hydrolysis of methyl acetate

Phase equilibria

a) Study of the variation of mutual solubility temperature with concentration for the phenol water system and determination of the critical solubility temperature.

Potentiometry: Potassium dichromate vs. Mohr's salt

Conductance

a) Determination of cell constant

b) Determination of equivalent conductance, degree of dissociation and dissociation constant of a weak acid.

References

1. J.B. Yadav, Advanced Practical Physical Chemistry, Goel Publishing House, **2001.**
2. G.W. Garland, J.W. Nibler, D.P. Shoemaker, Experiments in Physical Chemistry, 8th Edn. McGraw Hill, **2009.**
3. B. Viswanathan, Practical Physical chemistry, Viva Pub., **2005**

4. Practical Physical Chemistry Paperback, **1974** by A.M. James, F.E. Prichard.

Semester VI
Nuclear, Basic Organometallic & Bioinorganic Chemistry

Credit: 4 **Theory**

Objectives:

To introduce the concept of nuclear chemistry and origin of universe, principles of metallurgy, organometallic chemistry and its relevance in catalysis, and bioinorganic chemistry.

Learning Outcomes:

Ensures the students to gain the concept of evolution, chemistry of nuclear reactions, importance of metallurgy, structure, bonding and reactivity of organometallic complexes, and knowledge of bioinorganic chemistry in relation to living systems.

Nuclear Chemistry I: Introduction – composition of nucleus and nuclear forces. Nuclear stability – n/p ratio, mass defect, binding energy, packing fraction and magic numbers, shell and drop models. Isotopes – detection and separation. Isotopic constitution of elements and whole number rule. Deviation of atomic weights from whole numbers. Isobars, isotones and isomers.

Nuclear Chemistry II: Radioactivity – discovery, detection and measurements (Wilson cloud chamber). Radioactive emanations. Disintegration theory – modes of decay – Group displacement law – Rate of disintegration – Half life and average life – Radioactive series. Nuclear transformations – use of projectiles – nuclear reactions – fission and fusion. Nuclear reactors, radio-analytical techniques and activation analysis. Nuclear medicine. Applications of nuclear science in agriculture and medicine- carbon dating - rock dating - radioactive waste disposal.

General Principles of Metallurgy: Chief modes of occurrence of metals based on standard electrode potentials. Ellingham diagrams for reduction of metal oxides using carbon as reducing agent. Hydrometallurgy, Methods of purification of metals (Al, Pb, Ti, Fe, Cu, Ni, Zn): electrolytic, oxidative refining, Kroll process, Parting process, van Arkel-de Boer process and Mond's process. Preparation of metals (ferrous and nonferrous) and ultrapure metals for semiconductor technology.

Organometallic Compounds: Definition and Classification with appropriate examples based on nature of metal-carbon bond (ionic, s, p and multicentre bonds). Structures of methyl lithium, Zeise's salt and ferrocene. EAN rule as applied to carbonyls. Preparation, structure, bonding and properties of mononuclear and polynuclear carbonyls of 3d metals. π--acceptor behaviour of carbon monoxide. Synergic effects (VB approach)- (MO diagram of CO can be referred to for synergic effect to IR frequencies). Homogenous catalysis.

Bioinorganic Chemistry-I: A brief introduction to bioinorganic chemistry. Role of metal ions present in biological systems with special reference to Na^+, K^+ and Mg^{2+} ions: Na/K pump; Role of Mg^{2+} ions in energy production and chlorophyll. Biologically important coordination compounds - haemoglobin, myoglobin, carbonic anhydrase and vitamin B_{12} - Their structure and application. Role of Ca^{2+} in blood clotting, stabilization of protein structures and structural role (bones).

Prescribed Books

1. Huheey, J. E., Keiter, E. A., Keiter, R. L. and Medhi, O. K., Inorganic Chemistry - Principles of Structure and Reactivity, 4th edition, Pearson Education, **2006.**
2. Atkins, P., Overton, T., Rourke, J., Weller M., and Armstrong, F., Inorganic Chemistry, 5th edition, Oxford University Press, **2010**.
3. Lee, J. D., Concise Inorganic Chemistry, 5th edition, Wiley-India, **2010.** Lippard, S. J., and Berg, J. M., Principles of Bioinorganic Chemistry, Panima Publishing Company, New Delhi, **1997.**
4. Kaim W., and Schewederski, B., Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, John Wiley & Sons, New York, USA**, 2013.**
5. J. Chem. Education, 62, No. 11, **1985**
6. Arnikar, H. J., Essentials of Nuclear Chemistry, 4th edition, New Age International
7. Publishers Ltd., New Delhi, **1995.**
8. Loveland, W. D., Morrissey, D. J., Seaborg, G. T., Modern Nuclear Chemistry, Wiley- VCH Verlag GmbH Co. KGaA, **2006.**
9. Glasstone, Source Book on Atomic Energy, 3rd edition, Affiliated East West Press, **1979**.
10. BD Gupta and Anil J. Elias, Basic Organometallic Chemistry: Concepts, Syntheses, and Applications of Transition Metals, 1st edition, Universities Press, CRC Press, **2010.**
11. Crabtree, R. H., Organometallic Chemistry of the Transition Metals, Wiley, New York, **1988.**

Reference Books

1. Miessler, G. L., and Tarr, D. A., Inorganic Chemistry, 3rd edition, Pearson, **2004.**
2. Gilreath, E. S., Fundamental concepts of Inorganic Chemistry', International student's edition. Mcgraw-Hill Kogakusha, Ltd., **1958**.
3. Chatwal G., and Yadu, M.S., 'Coordination Chemistry', 1st edition, Himalaya Publishing House, **1992**.
4. Douglas, B., McDaniel, D., and J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd edition, John Wiley & Sons, **2010**.
5. Cotton, F. A., Wilkinson, G., Murillo, C. A., and Bochmann, M., Advanced Inorganic Chemistry, 6th edition, John Wiley & Sons, **2008**.
6. Day Jr, M. C., and Selbin, J. Theoretical Inorganic Chemistry, Literary Licensing, LLC, **2012**
7. Boyer, H. E., and Gall, T. L., Metals Handbook, Desk edition, **1984.**

Semester VI

Reaction Mechanisms & Natural Products Chemistry

Credit: 4 **Theory**

Specific objectives:

To introduce the advance organic reaction mechanisms, molecular rearrangements, synthetic organic transformations and the chemistry of biomolecules.

Learning outcomes:

Ensures the students to understand and acquire knowledge on advanced organic reaction mechanisms, molecular rearrangements, synthetic organic transformations and the chemistry of biomolecules (carbohydrates, terpenoids, alkaloids, vitamins and co-enzymes).

Organic transformations based on carbanions: Dicarboxylic acids, dicarbonyls, diesters, Acidity of α-hydrogens, alkylation of diethyl malonate and ethyl acetoacetate. Synthesis using diethyl malonate and ethyl acetoacetate, Claisen condensation. Knoevenagel condensation,

Molecular rearrangements: classification – electrophilic, nucleophilic and free radical rearrangements, mechanisms of the following rearrangements: pinacol-pinacolone, Wagner – Meerwin, Tiffenev-Demjanov, Dienone- Phenol, Favorskii, Hofmann, Schmidt, Lossen, Curtius, Beckmann, Fries, Baeyer –Villager, Stevens, Benzil – Benzilic acid, Brook and Benzidine, sommelet hauser rearrangement.

Natural products, biomolecules and biosynthesis:
Alkaloids: Occurrence, importance, general methods of structural elucidation - Structure and synthesis of nicotine and piperine, morphine, cocaine. Terpenes: Occurrence, importance, general methods of structural elucidation - classification, Isoprene rule, structure and synthesis of citral, geraniol and α-terpineol. Vitamins: Occurrence, importance - classification - Chemical constitution and physiological functions of vitamins A, B2 (Riboflavin), id).C (Ascorbic acid); Biosynthesis of natural products such as terpenes and alkaloids

Natural pigments: Flavones, flavanones, isoflavones, xanthones, quinones, pterins, chlorophyll and haemin.

Prescribed Books

1. Carey, F.A., Sundberg, R.J., Advanced Organic Chemistry, Part A: Structure and Mechanisms, 5th edn, Springer, **2007.**
2. Carey, F.A., Sundberg, R.J., Advanced Organic Chemistry, Part B: Reaction and Synthesis, 5th edn, Springer**, 2007.**
3. Smith M. B.,March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 7th edn, Wiley, **2015.**
4. Thomson, R.H., The Chemistry of Natural Products, 2nd edn, Springer, **1993.**

Reference Books

1. Finar, I.L. Organic Chemistry, Vol I, 6th edn, Pearson Education, **2002**
2. Finar, I.L. Organic Chemistry, Vol II, 5th edn, Pearson Education India, **2002**
3. Morrison, R.T., Boyd, R.N. Organic Chemistry, 7th edn, Pearson Education, **2010.**
4. Pine, S. H., Organic Chemistry, 5th edn, Tata McGraw Hill Education, **2006.**
5. Smith M. B.,March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 7th edn, Wiley, **2015.**
6. Carruthers, W., Coldham, I., Modern Methods of Organic Synthesis, 4th edn, Cambridge University Press, **2015.**
7. Clayden,J.,Greeves,N.,Warren.S.Organic Chemistry,2ndedn,Oxford University Press, **2014.**
8. Sykes, P. A Guidebook to Mechanism in Organic Chemistry, 6th edn, Pearson Education, **2003.**
9. Nelson, D. L., Cox, M. M. Lehninger's Principles of Biochemistry, 7th edn., WH Freeman, **2017.**

Semester VI
Quantum Chemistry & Molecular Spectroscopy

Credit: 4 **Theory**

Course Objective:

- To emphasis the Importance of quantum mechanics and its advantage over classical mechanics.
- To introduce the basis quantum mechanical postulates with the overview of Schrödinger equation.
- To apply the Schrödinger equation to solve one electron system. Further extended to He and Li
- To study the light-mater interaction using optical and resonance spectroscopy
- To understand the evolution, characteristics of various spectra

Course outcome:

After successful completion of this course, the students will able

- To understand the physical meaning of wave function and its application towards molecular modelling.
- To familiarize theoretical background of fundamentals of spectroscopy
- To co-relate molecular physical phenomena with spectral response

Quantum Chemistry I:

Classical mechanics and its disadvantages, Introduction to Quantum mechanical ideas: photoelectric effect, Compton effect, Black-body radiation, Atomic spectra.

Elements of Quantum mechanics: Postulates of quantum mechanics, wave functions, quantum mechanical operators and observables, Schrödinger equation.

Application of Schrodinger equation: Free particle and "particle-in-a-box" (rigorous treatment), quantization of energy levels, zero-point energy and Heisenberg Uncertainty principle; wave functions, probability distribution functions, nodal properties. Particle in a two and three dimensional boxes, separation of variables, degeneracy.

Qualitative treatment of simple harmonic oscillator model of vibrational motion: Setting up of Schrödinger equation and discussion of solution and wave functions. Vibrational energy of diatomic molecules and zero-point energy.

Angular momentum: Commutation rules, quantization of square of total angular momentum and z-component.

Rigid rotator model of rotation of diatomic molecule. Schrödinger equation, transformation to spherical polar coordinates. Separation of variables. Spherical harmonics. Discussion of solution.

Qualitative treatment of hydrogen atom and hydrogen-like ions: setting up of Schrödinger equation in spherical polar coordinates, radial part, quantization of energy (only final energy expression). Average and most probable distances of electron from nucleus. Schrödinger equation for many-electron atoms (He, Li).

Molecular Spectroscopy I:

Interaction of electromagnetic radiation with molecules and various types of spectra; Born-Oppenheimer approximation.

Rotation spectroscopy: Selection rules, intensities of spectral lines, determination of bond lengths of diatomic and linear triatomic molecules, isotopic substitution.

Vibrational spectroscopy: Classical equation of vibration, computation of force constant, amplitude of diatomic molecular vibrations, anharmonicity, Morse potential, dissociation energies, fundamental frequencies, overtones, hot bands, degrees of freedom for polyatomic molecules, modes of vibration, concept of group frequencies. Fingerprint region, Fermi resonance.

Raman spectroscopy: Qualitative treatment of Rotational Raman effect; Effect of nuclear spin, Vibrational Raman spectra, Stokes and anti-Stokes lines; their intensity difference, rule of mutual exclusion.

Electronic spectroscopy: Franck-Condon principle, electronic transitions, singlet and triplet states, fluorescence and phosphorescence, dissociation and predissociation, calculation of electronic transitions of polyenes using free electron model.

Nuclear Magnetic Resonance (NMR) spectroscopy: Principles of NMR spectroscopy, Larmor precession, chemical shift and low resolution spectra, different scales, spin-spin coupling and high resolution spectra.

Electron Spin Resonance (ESR) spectroscopy: Its principle, hyperfine structure, ESR of simple radicals.

Reference Books

1. R.K. Prasad, Quantum Chemistry, New Age International, **2001**
2. Lowe, J. P. & Peterson, K. Quantum Chemistry, Academic Press **2005**.
3. Mc Quarrie, J. D. Simon, Physical Chemistry – A molecular Approach, Viva Books.
4. I.N. Levine, Physical Chemistry, Tata McGraw Hill,
5. Gurdeep Raj, Advanced Physical Chemistry, Goel Publishing House
6. Banwell, C. N. &Mc Cash, E. M. Fundamentals of Molecular Spectroscopy,4th Ed. Tata McGraw-Hill: New Delhi **2006**.
7. Manas Chanda, Atomic structure and Chemical bonding in Molecular Spectroscopy" Tata McGraw Hill.
8. D. L. Pavia, G. M. Lampman, G. S. Kriz, Introduction to spectroscopy, 3rd edn, Thomson Brooks/Cole, **2001**.
9. D. N. Satyanarayana, Electronic absorption spectroscopy and related techniques, Universities Press.
10. D.N. Sathyanarayana, Introduction to Magnetic Resonance Spectroscopy ESR, NMR, NQR, IK International, **2009**.
11. Puri, Sharma & Pathania, Principles of Physical Chemistry, Vishal Publishing Co.

Semester VI
Analytical & Inorganic Chemistry Laboratory II

Credit: 2 **Practical**

Objectives

To apply the knowledge of analytical technique to separate mixture of alkaline earth metals and transition metals of various oxidation state with the help of Hard-soft acid base theory

Learning Outcomes

Ability to separate the mixture of cations (common and rare cations) by semi-micro qualitative analysis

Semi-micro qualitative analysis of a mixture containing two common and two rare - cations.

Reference Books:

1. Svehla, G. Vogel's Qualitative Inorganic Analysis, Pearson Education, **2012**.
2. Mendham, J. Vogel's Quantitative Chemical Analysis, Pearson, **2009**.
3. Ghoshal, Mahapatra and Nad, An Advanced Course in Practical Chemistry, New Central Book Agency, **2011**.
4. Venkateswaran V. Veerasamy R. Kulandaivelu A.R., Basic principles of Practical Chemistry, 2nd edition, New Delhi, Sultan Chand & sons, **1997**.

Semester VI
Organic Chemistry Laboratory III

Credit 2 **Practical**

Specific objectives:
To introduce the experimental aspects of organic chemistry involving different synthetic methods followed by isolation and characterization of organic compounds.

Learning outcomes:
Students will learn various experimental organic techniques involving functional group transformations, isolation and characterization.

1. Preparations:
Two-step preparations (any three) involving acetylation, methylation, condensation, rearrangements and photochemical reactions.

2. Isolation and characterization of natural products:

a) Isolation of caffeine from tea dust
b) Isolation of casein from milk
c) Isolation of piperine from pepper
d) Isolation of lycopene from tomato

Reference Books

1. Vogel, A.I., Tatchell, A.R., Furnis, B.S., Hannaford, A.J., Smith, P.W.G., Textbook of Practical Organic Chemistry, Prentice-Hall, 5th edn, **1996**.
2. Mann, F.G., Saunders, B.C. Practical Organic Chemistry, 4th edn, Pearson Education India, **2009**.
3. Khosla, B. D.; Garg, V. C. & Gulati, A. Senior Practical Physical Chemistry, R. Chand & Co.: New Delhi **2011**.
4. Qualitative Organic Analysis, Quantitative Organic Analysis, Pearson Education, **2011**.
5. Leonard, J., Lygo, B., Procter. G., Advanced Practical Organic Chemistry, 3rd edn, CRC Press, **2013**.
6. Cranwell, P. B., Harwood, L. M., Moody, C. J., Experimental Organic Chemistry, 3rd edn, Wiley-Blackwell**, 2017**.
7. Ahluwalia, V.K., Aggarwal, R. Comprehensive Practical Organic Chemistry, Universities Press, **2004**.

Semester VI
Physical Chemistry Laboratory III

Credit: 2 **Practical**

Course objective

- To get hands-on experience on quantum mechanical and computational methods.
- To perform single point/geometry optimization of various organic and inorganic compounds.
- To introduce various UV-Visible spectroscopy methods and its applications.

Course outcome

After successful completion of this course, the students will able

- To model the organic/inorganic compounds in their ground state electronic configuration.
- To evaluate and study the energy, concentration, structures and kinetics using various spectroscopic methods.

Quantum Mechanics:

1. Optimization of Geometry and single point energy calculations of Organic molecules
2. Calculation of energy gap between HOMO and LUMO in simple molecules and visualization of molecular orbitals
3. Calculation of dipole moment in polar organic molecules.
4. Prediction of the stability of ortho, meta, para products of nitration of aromatic ring using computational chemistry calculations.
5. Calculation of IR stretching frequencies of groups and visualization of normal modes of vibration in organic molecules.

Spectroscopy:

1. Study the 200-500 nm absorbance spectra of $KMnO_4$ and $K_2Cr_2O_7$ (in 0.1 M H_2SO_4) and determine the λmax values. Calculate the energies of the two transitions indifferent units (J molecule^{-1}, kJ mol^{-1}, cm^{-1}, eV).
2. Study the pH-dependence of the UV-Vis spectrum (200-500 nm) of $K_2Cr_2O_7$.
3. Record the 200-350 nm UV spectra of the given compounds (acetone, acetaldehyde,2-propanol, acetic acid) in water. Comment on the effect of structure on the UV spectra of organic compounds.
4. Verify Lambert-Beer's law and determine the concentration of $CuSO_4$/$KMnO_4$/ $K_2Cr_2O_7$ in a solution of unknown concentration
5. Determine the concentrations of $KMnO_4$ and $K_2Cr_2O_7$ in a mixture.
6. Study the kinetics of iodination of propanone in acidic medium.
7. Determine the amount of iron present in a sample using 1,10-phenathroline.
8. Determine the dissociation constant of an indicator (phenolphthalein).
9. Study the kinetics of interaction of crystal violet/ phenolphthalein with sodium hydroxide.

10. Analyse the given vibration-rotation spectrum of HCl(g)

Reference Books

1. J. Foresman & Aelieen Frisch, Exploring Chemistry with Electronic Structure Methods, Gaussian Inc., 2000.
2. D.C. Young, Computational Chemistry: A Practical Guide for Applying Techniques to Real World Problems, John Wiley & Sons, 2001.
3. D. Rogers Computational Chemistry Using the PC, 3rd Edition, John Wiley & Sons (2003).
4. A. Leach, Molecular Modelling: Principles and Applications, 2nd Edn, Longman, 2001.
5. J. M. Haile (2001) Molecular Dynamics Simulation: Elementary Methods.
6. J.B. Yadav, Advanced Practical Physical Chemistry, Goel Publishing House, 2001.
7. G.W. Garland, J.W. Nibler, D.P. Shoemaker, Experiments in Physical Chemistry, 8th Edn. McGraw Hill, 2009.
8. Saroj Kumar and Naba Kumar, Physical Chemistry Practical, New Central Book Agency,2012

Semester VII
Solid State, Main Group & Coordination Chemistry

Credit: 4 **Theory**

Objectives:

To introduce the concept of solid state chemistry, structural diversity of the main group elements, and advanced level of coordination chemistry and its multitudes of applications.

Learning Outcomes:

Ensures the students to gain the concept of solid state chemistry, understand the structure and properties relationship of the main group elements, coordination chemistry and reaction mechanisms.

Synthesis and modification of inorganic solids: Structures of ionic crystals – AX and AX_2 type crystal structures – layer structures - lattice energy - Born-Lande, Born-Mayer and Kapustinskii equations – Derivations and applications –Review of defects in ionic solids - Thermodynamic effects of defects. Band theory, n- and p- type semiconductors and superconductors. Reactions in solid state - diffusion, diffusion coefficient, diffusion mechanisms, vacancy and interstitial diffusion, thermal decomposition of solids -Type I and Type II reactions. Phase Transitions - classification of phase transitions-first and second order phase transitions, Martensitic transformations, order-disorder transitions. Conventional heat and beat methods, Co-precipitation method, Sol-gel methods, Hydrothermal method, Ion-exchange and Intercalation methods. Molecular material and fullerides, molecular materials & chemistry – one-dimensional metals, molecular magnets, inorganic liquid crystals.

The Chemistry of the Main Group Elements: Inorganic Rings, chains, and cages Catenation and Heterocatenation, Heterocyclic ring system- Borazines, Phosphazines-

Monomer and Polymer, S-N ring compounds, Homocyclic rings of S, Se and Te. Silicate minerals, Isopolyanions, Boranes: boron cage compounds-closo, nido, arachno, carboranes; cage compounds of S and P. Metal cluster: metal-metal bonding and reactivity of di-, tri- and polynuclear clusters.

Coordination Chemistry II: Recapitulation of Crystal field theory - splitting of d-orbitals under various geometries - Limitations of CFT – Ligand field Theory - MO theory – sigma – and pi-bonding in complexes and evidences for π-bonding – nephelauxetic effect – angular overlap model. Studies of coordination compounds in solution – detection of complex formation in solution – Stability constants – stepwise and overall formation constants – simple methods (Potentiometric, pH metric and photometric methods) of determining the formation constants - factors affecting stability – Irving-William series -statistical and chelate effects – forced configurations.

Coordination Chemistry-III: Reaction Mechanism: Kinetics and mechanism of reactions in solution – labile and inert complexes – ligand displacement reactions in octahedral and square planar complexes – acid hydrolysis, base hydrolysis and anation reactions – trans effect – theory and applications. Electron transfer reactions – complementary and non-complementary types – inner sphere and outer sphere processes – Excited state outer sphere electron transfer reactions - isomerisation and racemisation reactions of complexes – reactions of four and six-coordinate complexes – interconversion between stereoisomers.

Prescribed Books

1. Huheey J. E., Keiter E. A. and Keiter R. L. and Medhi O. K., Inorganic Chemistry - Principles of Structure and Reactivity, 4th edition, Pearson Education, **2006**.
2. Atkins, P. W.; Paula, J.; Physical Chemistry, Oxford Publications, 8th edition, **2009**.
3. B. Douglas, D. McDaniel and J. Alexander, Concepts and Models of Inorganic Chemistry,3rd edition, John Wiley & Sons, **2010**.
4. F. A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, 3rd ed. Wiley-Eastern Company, New Delhi, **1990**.
5. Azaroff, L.V., Introduction to Solids, McGraw hill, New York. **1960.**
6. West, A. R., Solid State Chemistry and Its Applications, John Wiley & Sons, **1984**.
7. Chakrabarty, K., Solid State Chemistry, New Age Publishers, **1996.**
8. Keer, H. V., Principles of the Solid State, Wiley Eastern Limited, **1993**.
9. D.M. Adams, Inorganic Solids: An Introduction to Concepts in Solid State Structural Chemistry, Wiley, **1974**.
10. C.N.R. Rao, K.J. Rao, Phase Transitions in Solids, McGraw Hill, **2010**.
11. A.Earnshaw, Introduction to Magnetochemistry, Academic Press, **1968**.

Reference Books

1. Day, M. C., and Selbin, J., Theoretical Inorganic Chemistry, Affiliated East West Press Pvt. Ltd. 2nd edition,**1985**.

2. Kettle, S. F. A., Physical Inorganic Chemistry – A Coordination Chemistry Approach, Spectrum Academic Publishers, Oxford University Press, **1996**.
3. Basolo, F., and Pearson, R. G., Mechanism of Inorganic Reactions, John Wiley, New York,**1967**.
4. Miessler, G. L., and Tarr, D. A., Inorganic Chemistry, 3rd edition, Pearson, **2004**. Housecraft, C. E., and Alan G. Sharpe, Inorganic Chemistry, 4th edition, Pearson, **2012**.
5. Purcell, K. F., and Kotz, J. C., Inorganic Chemistry, Cengage Learning, **2012**.Day Jr ,M. C., and Selbin, J, Theoretical Inorganic Chemistry, Literary Licensing,LC, **2012**
6. Wilkinson, G., Gillars, R. D., and Mccleverty, J. A., Comprehensive Co-ordination Chemistry, Pergamon Press, **1987**.
7. Wulfberg, G., Inorganic Chemistry, University Science Books, **2000**.
8. Adam, D.M. Inorganic Solids: An introduction to concepts in solid-state structural chemistry. John Wiley & Sons, **1974**
9. Rodger, G.E. Inorganic and Solid State Chemistry, Cengage Learning India, Edition, **2002**.

Semester VII
Physical Organic Chemistry & Aromatic Compounds

Credit: 4 **Theory**

Specific objectives:

To introduce the advanced level concepts in stereochemistry, aromaticity, heterocyclic compounds and physical organic chemistry.

Learning outcomes:

Ensures the students to understand, acquire knowledge on topicity, asymmetric synthesis, determining the reaction mechanisms by different methods, criteria for aromaticity in non benzenoid molecules and other advanced polycyclic aromatics and the nomenclature and reactions of complex heterocyclic.

Advanced Stereochemistry: Configuration - conformation of cycloalkanes, conformation and reactivity -stereochemistry of allenes, spiranes, biphenyls, molecules with chiral planes, Topicity stereoselective and stereospecific reactions - enantioselective reactions - double stereo differentiation, asymmetric synthesis, chiral auxiliaries, chiral catalysts and reagents.

Physical organic chemistry: Thermodynamic stability – general relationship between thermodynamic stability and reaction rates – electronic substituent effects on reaction intermediates – kinetic isotope effects – linear free energy relationships – principles of microscopic reversibility – substituent effects – solvent and solvent effects – methods of determination of reaction mechanism.

Aromaticity: Criteria of aromaticity - Craig's rule – non-benzenoid aromatic compounds – anti-aromaticity, homoaromaticity – fused-ring systems –hetero aromatic systems.

Nucleophilic aromatic substitution reactions – VNS - transition metal- catalyzed aromatic substitution reactions – aromatic substitution reactions involving radical intermediates.

Advanced Heterocycles: Nomenclature, heterocyclics with two hetero atoms – fused five and six membered heterocyclics – preparation and reactions of indole, quinoline, isoquinoline and carbozole.

Prescribed books

1. Carey, F.A., Sundberg, R.J., Advanced Organic Chemistry, Part A: Structure and Mechanisms, 5th edn, Springer, **2007**.
2. Carey, F.A., Sundberg, R.J., Advanced Organic Chemistry, Part B: Reaction and Synthesis, 5th edn, Springer, **2007**
3. Nasipuri, D., Stereochemistry of Organic Compounds: Principles and Applications, 4th edn, New Academic Science Publisher, **2012**.
4. Eliel, E. L., and Wilen, S. H. Stereochemistry of Organic Compounds, Wiley, **1994**.
5. Joule, J.A., Mills, K, Heterocylic Chemistry, 5th edn, Wiley-Blackwell, 2010.
6. Bansal, R. K., Heterocyclic Chemistry, 5th edn, New Age International Private Limited, **2017**

Reference books

1. Morrison, R.T., Boyd, R.N. Bhattacharjee, S. K., Organic Chemistry, 7th edn, Pearson Education, **2010**.
2. Pine, S. H., Organic Chemistry, 5th edn, Tata McGraw Hill, **2008.**
3. Carruthers, W., Coldham, I., Modern Methods of Organic Synthesis, 4th edn, Cambridge University Press, **2015**.
4. Smith M. B.,March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 7th edn, Wiley, **2015**
5. Finar, I.L. Organic Chemistry, Vol I, 6th edn, Pearson Education, **2002**
6. Sykes, P. A Guidebook to Mechanism in Organic Chemistry, 6th edn, Pearson Education, **2003**.
7. Kalsi, P. S., Stereochemistry: Conformation and Mechanism, 9th edn, New Age International Private Limited, **2017**
8. Katritzky, A, R., Ramsden, C. A., Joule, J. A., Zhdankin, V. V., Handbook of Heterocyclic Chemistry, 3rd edn, Elsevier, **2010**.
9. Anslyn, E. V., Dougherty, D. A., Modern Physical Organic Chemistry, University Science Books**, 2005**

Semester VII
Chemical Kinetics & Group Theory

Credit: 4 **Theory**

Course objective

- To introduce the essential concepts of chemical kinetics; important postulates and theories.
- To familiarize about the widely applicable enzyme catalysis and its mechanism.
- To predict the kinetics of Rice – Herzfeld mechanisms and explosive reactions.
- To give an overview of Group theory, Symmetries, Optical Activity, Dipole Moment and Irreducible Representations.
- To apply Applications of symmetry concepts in Spectroscopies and Chemical Bonding.

Course outcome

After successful completion of this course, the students will able

- To use various experimental techniques to determine the kinetics of chemical reactions.
- To determine the overall symmetry of any small and medium-sized molecule and apply concept of point group and GOT to study their chemical properties.

Chemical Kinetics

Reaction rates and order of reactions, determination of order of reactions, complex reactions, reversible, consecutive and concurrent reactions. Reactions of variable order- steady state treatment, free radical reactions-the Rice Herzfeld Mechanism.

Fast reactions: relaxation, Flow and Shock methods, Molecular beam methods Flash photolysis. Introduction to femtochemistry

Theories of reaction rates: Arrhenius equation, Collision cross section and reaction cross section. -steric factor, potential energy surfaces, Thermodynamic formulations of Collision & Transition state theories Comparative study of the theories of reaction rates. Thermodynamic treatment of Reaction rates, Effect of pressure on velocity of gas reactions. Molecular Reaction Dynamics: Heterogeneous catalysis: Unimolecular and bimolecular surface reactions, Langmuir-Hinshelwood and Langmuir-Rideal mechanism-ARRT of surface reactions,

Enzyme catalysis: Michelis-Menten equation, effect of pH and temperature on enzyme catalysis.

Eley-Rideal and Hinshelwood mechanisms, Lindemann-Hinshelwood mechanism, qualitative idea of RRKM theory, chain reactions, steady state treatment (kinetics of H_2-Cl_2 and H_2Br_2 reactions), Rice – Herzfeld mechanism, Explosive Reactions H_2-O_2 (Semenov-Hinshelwood)

Group Theory

Symmetry: Fundamentals Concept of Symmetry, Matrix representation of symmetry operations. concepts of groups, molecular point groups, representation of groups, matrix representation of symmetry operations, reducible and irreducible representations, Symmetry criterion of optical activity, symmetry restrictions on dipole moment.

Great Orthogonality Theorem: Interpretation of character tables. Determination of symmetry species for translations and rotations.

Vibrational spectra: transition moment integral, vanishing of integrals, symmetry aspects of molecular vibrations, vibrations of polyatomic molecules-selection rules for vibrational absorption. Symmetry of normal modes of H_2O, C_2H_4, Trans-N_2F_2, $CHCl_3$and NH_3 using Cartesian coordinates and internal coordinates.

Applications in Spectroscopy

I. Complementary nature of IR and Raman spectra-determination of the IR and Raman active vibrational modes
II. Electronic spectra: selection rules for electronic transition, electronic transitions simple aldehydes

Applications in chemical bonding

I. Transformation of atomic orbitals- Symmetry adapted linear combinations (SALC), Construction of hybrid orbitals for AB_3(planar), AB_4(Td), AB_5(D_3h) and AB_6(Oh) type of molecules
II. Ligand field theory-splitting of d orbitals in different environments using group theoretical considerations
III. MO diagram for water and ammonia, method of descending symmetry

Reference Books

1. W. J. Moore and R. G. Pearson, Kinetics and Mechanism, Wiley, New York, **1988**
2. F. Daniels and R. A. Alberty, Physical Chemistry, 8h Edition, Wiley, New York, **1994**
3. P. W. Atkins, Physical Chemistry 8th Edn., Wiley, New York, **2006**
4. J. Rajaram, J.C. Kuriakose, Kinetics and Mechanisms of Chemical Transformations, Macmillan India, **2000.**
5. K.J. Laidler, Chemical kinetics, 3rd Edn. Harper & Row**, 1987.**
6. C. Kalidas, Chemical Kinetic Methods: Principles of Fast Reaction Techniques and Applications, New Age International**, 2005.**
7. D.A. McQuarrie, J. D. Simon, Physical chemistry: A Molecular Approach, University Science Books,**1997**
8. F. A. Cotton: Chemical Applications of Group Theory, Wiley Eastern, **1985.**
9. P. K Ghosh and P. K Shukla:Atomic Electronic Structure, Prentice Hall of India,**1994.**
10. V. Ramakrishnan and M. S. Gopinathan: Group Theory in chemistry, Vishal Publication, **1986.**
11. D. M. Bishop, Group theory and Chemistry, Dover, **1989.**

Semester VII
Advanced Organic Chemistry Laboratory

Credit: 4 **Practical**

Specific objectives:

To introduce the experimental aspects of advanced organic chemistry involving multistep synthesis, qualitative and quantitative analysis of organic compounds.

Learning outcomes:

Ensures the students to understand, acquire knowledge and have hands on experience in multistep organic synthesis and analysis by using spectroscopic techniques. Separation techniques and functional group analysis.

1. Multistep organic synthesis (any four) - conventional synthesis - microwave assisted synthesis - photochemical reactions. Purification of the compounds using column chromatography and characterization of the compounds using spectroscopic techniques.

2. Qualitative Analysis: Separation and analysis of organic mixture containing two components and preparation of suitable derivatives (at least four compounds).

3. Estimation of organic compounds:

   a) Estimation of phenol and aniline - volumetric method.
   b) Estimation of glucose by Betrands method.
   c) Estimation of methyl ketone – iodimetric method
   d) Differentiation between a reducing and a nonreducing sugar.
   e) Determination of iodine and saponification value of an oil sample.

Prescribed Books

1. Vogel, A. I., Elementary Practical Organic Chemistry: Small Scale Preparations, Qualitative Organic Analysis, Quantitative Organic Analysis, Pearson Education, **2011**.
2. Ahluwalia, V.K., Aggarwal, R. Comprehensive Practical Organic Chemistry, Universities Press, **2004**
3. Bansal R. K., Laboratory Manual in Organic Chemistry, New Age International Pvt. Ltd Publishers, **2009**.
4. Mann, F.G., Saunders, B.C. Practical Organic Chemistry, 4th edn, Pearson Education India, **2009**
5. Vogel , A.I., Tatchell, A.R., Furnis , B.S., Hannaford , A.J., Smith, P.W.G., Vogel's Practical Organic Chemistry, 5th edn, Pearson education Ltd, **1996**.

Reference Books

1. Leonard, J., Lygo, B., Procter. G., Advanced Practical Organic Chemistry, 3rd edn, CRC Press, **2013**.
2. Cranwell, P. B., Harwood, L. M., Moody, C. J., Experimental Organic Chemistry, 3rd edn, Wiley-Blackwell, **2017**.

Semester VIII
Advanced Organometallic & Bioinorganic Chemistry

Credit: 4 **Theory**

Specific objectives:

To the concepts of organometallics, bonding, structure, reaction mechanism and catalysis and to introduce the principles of bioinorganic chemistry

Learning outcomes:

Upon successful completion of this course, the student should be able to:

- Ensures the students to understand, acquire knowledge on ligands and fluxional molecules, different organic ligands and metal complexes, reaction mechanism and catalysis.
- Understand the concepts of Bioinorganic Chemistry.
- Understand the function and transport of Alkali and Alkaline earth metals in the biological systems.
- Describe the important roles of metal ions in metalloproteins/metalloenzymes.
- Identify the appropriate analytical techniques that are useful in characterizing transition-metal coordination in biological molecules.
- Understand the importance of metal ions ion medicine.

Structure and bonding in organometallics: 16/18-Electron rule - metal carbonyls – bonding –spectra – metal alkyls, aryls, hydrides and dihydrogen complexes - ligands – metallocenes - electronic structure and bonding in ferrocene - synthesis, physical and spectroscopic properties of metallocenes – fluxional molecules.σ–bonded ligands: metal-phosphines / metal- nitrosyls: structures, reactivity and bonding. Carbenes: N-heterocyclic carbenes, Fischer carbenes, Schrock carbenes, carbynes. Isolobal analogy, metal-metal bond, transition metal clusters. Quintuple bond.

Reaction mechanism and catalysis: oxidative addition, reductive elimination, insertion, hydride elimination, abstraction; hydrogenation of olefins, hydroformylation, Wacker process, Ziegler-Natta polymerisation, cyclo oligomerisation, Isomerization reactions, olefin metathesis, Monsanto acetic acid synthesis, Fischer-Tropsch process, hydrosilylation, carbonylation, and CH functionalization reactions.

Bioinorganic Chemistry II: Metalloporphyrins/Metalloenzymes

Metals at the Center of Photosynthesis: Primary Processes in Photosynthesis – Photosystems I and II - Light Absorption (Energy Acquisition) – Exciton transport (Direct Energy Transfer) – Charge separation and electron transport – Manganese catalyzed oxidation of water to O_2.

Dioxygen transport and storage - hemoglobin and myoglobin: electronic and spatial structures - hemerythrin and hemocyanine – synthetic Oxygen carriers, model systems - blue copper proteins (Cu) - iron-sulfur proteins (Fe) - cytrochromes electron transport chain - carbon monoxide poisoning - iron enzymes - peroxidase, catalase and cytochrome P-450, copper enzymes - superoxide dismutase, carboxypeptidase, carbonicanhydrase, vitamin B_{12} and B_{12} coenzymes, nitrogen fixation. Medicinal bioinorganic chemistry: platinum complexes in cancer therapy – cis-platin and its mode of action – metal toxicity.

Magnetic properties: Types of magnetism – Dia –para – ferro and antiferro magnetism. Magnetic properties of free ions – first order Zeeman effect – Second order Zeeman effect – states KT – states<<KT. Determination of Magnetic moments and their applications to the elucidation of structures of inorganic compounds – temperature dependent and temperature independent paramagnetism - Magnetic properties of lanthanides and actinides. Spin crossover in coordination compounds.

Prescribed Books

1. Powell, P., Principles of Organometallic Chemistry, 2nd ed., Springer, 1998.
   Purcell, K. F., and Kotz, J. C., Inorganic Chemistry, Saunders Golden Sunburst Series, W.B. Saunders Company, Philadelphia, 1977.
2. Huheey, J. E., Keiter, E. A. and Keiter, R. L. and Medhi, O. K., Inorganic Chemistry - Principles of Structure and Reactivity,4th edition, Pearson Education, 2006.
3. Mehrotra, R. C., and Singh, A., Organometallic Chemistry, a Unified Approach, New Age International, 2006.
4. Crabtree, R. H., Organometallic Chemistry of the Transition Metals, Wiley, New York, 1988.
   Gupta, B. D., and Elias, Anil. J., Basic Organometallic Chemistry: Concepts, Syntheses, and Applications of Transition Metals, 1st edition, Universities Press, CRC Press, 2010.
5. Lippard, S. J., and Berg, J. M., Principles of Bioinorganic Chemistry, Panima Publishing Company, New Delhi, 1997.
6. Kaim W., and Schewederski, B., Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, John Wiley & Sons, New York, USA, 2013.
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8. S. P. Banerjee, Advanced Inorganic Chemistry, Arunabha Sen, Books and Allied (P) LTD. Volume II, 2015.

Reference Books

1. Elschenbroich, C., and Salzer, A., Organometallics: A Concise Introduction, 3rd edition, 1999.
2. Greenwood, N. N., and Earnshaw, A., Chemistry of the Elements, 2nd edition, Elsevier, 2005.
3. Jolly, W. L., Modern Inorganic Chemistry, McGraw Hill, New York, 2nd Edition, 1991.
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5. Douglas, B., McDaniel, D. H., and Alexander, J. J., Concepts and Models of Inorganic Chemistry, 2nd edition, John Wiley & sons, New York, 2006.
6. Bochmann, M., Organometallics 1: Complexes with transition metal-carbon s-bonds; Oxford Chemistry Primers Series,No. 13 Oxford Chemistry Primers Series, No.12, 1994.; Bochmann, M., Organometallics 2:Complexes with transition metal carbon π bonds, 1994.
7. Collman, J. P., Hegedus, L. S., Nortan, J. R. and Finke, R. G., Principles and Applications of Organotransition Metal Chemistry, University Science Books. Mill Valley, California, 1987.
8. R. H. Crabtree, Organometallic Chemistry of the Transition Metals, Wiley, New York,1988.
9. W. Parkins and R. C. Poller, An Introduction to Organometallic Chemistry
10. Haiduc and J. J. Zuckerman, Basic Organometallic Chemistry
11. R. Hoffmann, Angew. Chem. Int. Ed., Engl. 21, 711-800 1982.
12. BD Gupta and Anil J. Elias, Basic Organometallic Chemistry: Concepts, Syntheses, and Applications of Transition Metals, 1st edition, Universities Press, CRC Press, 2010.
13. Cotton, F. A., Wilkinson, G., Carlos A. Murillo, Manfred Bochmann, Advanced Inorganic Chemistry, 6th ed., A Wiley - Interscience Publication, John –Wiley & Sons, USA, 2007. Chem. Education, 62, No. 11, Bioinorganic Chemistry, State of the Art. 1985.
14. Eichorn, G. L., Inorganic Biochemistry, Volumes 1 & 2, 2nd ed., Elsevier Scientific Publishing Company, New York, 1973.
15. Atkins, P., Overton, T., Rourke, J., Weller M., and Armstrong, F., Inorganic Chemistry, 5th edition, Oxford University Press, 2010.

Semester VIII

Organic Photochemistry & rearrangements

Credit: 4 **Theory**

Specific objectives:

To introduce the concepts of photochemistry, pericyclics, rearrangements and name reactions.

Learning outcomes:

Ensures the students to understand, acquire knowledge on pericyclic reactions, organic photochemistry, molecular rearrangement and name reactions and their further applications in organic synthesis.

Pericyclic Reactions: Pericyclic reactions – orbital correlation diagram – FMO. Diels-Alder reactions – 1,3-dipolar cycloaddition reactions – [2+2] cycloadditions and related reactions leading to cylcobutanes – [3,3] and [2,3]-sigmatropic rearrangements – unimolecular thermal elimination reactions.

Organic photochemistry: Photochemistry of alkenes, dienes and polyenes – photochemistry of carbonyl compounds – photoreductions, photooxidations and photorearrangement reactions - photochemistry of aromatic compounds.

Molecular Rearrangements: Applications of molecular rearrangement reactions in the synthesis of complex organic molecules and natural products.

Selected name reactions in organic synthesis: Julia olefination; Baylis-Hillman reaction, Henry reaction, Nef reaction, Kulinkovich reaction, Ritter reaction, Sakurai reaction, Tishchenko reaction and Ugi reaction, Nazarov cyclization, Robinson annulation; McMurray reaction; Darzens reaction; Mitsunobu reaction; Dotz reaction;

Prescribed books

1. Carey, F. A., Sundberg, R. J., Advanced Organic Chemistry, Part B: Reaction and Synthesis, 5th edn, Springer, 2007.
2. Fleming, I,, Pericyclic Reactions, 2nd edn, Oxford University Press, Oxford, 2015.
3. Sankararaman, S., Pericyclic Reactions - Applications and Theory, Wiley – VCH, 2005.
4. Turro , N. J., Scaiano, J. C., and Ramamurthy, V., Modern Molecular Photochemistry of Organic Molecules, University Science Books, 2010
5. Sanyal and Sanyal, Reactions, Rearrangements and Reagents, 4th edn, Bharati Bhawan Publishers and Distributors; 2003
6. Singh, J., Photochemistry and Pericyclic Reactions, 3rd edn, New Age International Publishers, 2012.

Reference books

1. Morrison, R.T., Boyd, R.N. Bhattacharjee, S. K., Organic Chemistry, 7th edn, Pearson Education, 2010.
2. Pine, S. H., Organic Chemistry, 5th edn, Tata McGraw Hill, 2008.
3. Smith M. B.,March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 7th edn, Wiley, 2015
4. Finar, I.L. Organic Chemistry, Vol I, 6th edn, Pearson Education, 2002
5. Finar, I.L. Organic Chemistry, Vol II, 5th edn, Pearson Education India, 2002
6. Sykes, P. A Guidebook to Mechanism in Organic Chemistry, 6th edn, Pearson Education, 2003
7. Mukherjee, S.M., Singh, S.P., Reaction Mechanism in Organic Chemistry, Trinity Press, 2014.
8. Lowry, T. H., Richardson, K. S., Mechanism and Theory in Organic Chemistry, 3rd edn, Addison – Wesley Longman Inc., 1998.
9. Li, J. J., Corey, E. J., Name Reactions for Homologation, Part 1, Wiley-Blackwell, 2009
10. Mundy, B. P., Ellerd, M G., Favaloro Jr. F. G., Name Reactions and Reagents in Organic Synthesis, 2nd edn, Wiley-Blackwell, 2005
11. Carruthers, W., Coldham, I., Modern Methods of Organic Synthesis, 4th edn, Cambridge University Press, 2015.

Semester VIII
Advanced Quantum Chemistry & Molecular Spectroscopy

Credit: 4 **Theory**

Course objective:

- To solve Schrodinger equation for the most significant and elementary molecules using basic perturbation-variation principles and advanced VB-MO theories.
- To use the concept of LCAO to hybridization and directed bonding in polyatomic molecules.
- To introduce pulse sequences in magnetic resonance spectroscopy to avoid complexity in spectroscopy.
- To explain the basic principles and components of advanced molecular spectroscopy tools.

Course outcome:

After successful completion of this course, the students will able

- To understand recent computational chemistry and spectroscopic problems.
- Stepping stone to theoretical/Molecular spectroscopy/computational chemistry research

Quantum Chemistry II

Translational motion: free particle in one-dimension, particle in a 1-D box with infinite & finite potential walls, tunneling, particle in a 3-D box. Nonplanar rigid rotor (or particle on a sphere)- separation of variables, the phi and the theta equations and their solutions,

Legendre and associated Legendre polynomials. Spherical harmonics (imaginary and real forms) - polar diagrams of spherical harmonics.

Vibrational motion**:** 1-D harmonic oscillator (complete treatment), Hermite equation (solving by method of power series), Hermite polynomials, recursion relation, wave functions and energies-important features, Harmonic oscillator model and molecular vibrations.

Potential energy of hydrogen-like systems. The wave equation in spherical polar coordinates: separation of Variables-R, theta and phi equations and their solutions, wave functions and energies of hydrogen-like atoms. Orbitals-radial functions, radial distribution functions, angular functions and their plots. The postulate of spin by Uhlenbeck and Goudsmith, discovery of Spin-Stern Gerlach experiment. Spin orbitals-construction of spin orbitals from orbitals and spin functions.

Quantization of angular momentum, quantum mechanical operators corresponding to angular momenta (Lx, Ly, Lz and L^2)-commutation relations between these operators. Spherical harmonics as eigen functions of angular momentum operators Lz and L^2. Ladder operator method for angular momentum. Space quantization.

Schrödinger equation for Helium atom. Perturbation theory, Variational methods, Hartree-Fock equations, Self-consistent field methods for solving Hartree-Fock equations, Born-Oppenheimer approximation-molecular Hamiltonian operators, Valence bond treatment for chemical bonding in molecules, molecular orbitals, molecular orbital theory for different diatomic molecular systems, photoelectron spectra, SCF-LCAO-MO wave functions, electronic states of diatomic molecules, sp, sp^2 and sp^3 hybrid orbitals, molecular term symbols, Hückel molecular orbitals, bonding in polyatomic molecules.

EMR & Origin of spectra: Nature of EMR, Interaction of EMR with matter, Natural line width and intensity of spectral lines, Classical and quantum chemical approach to absorption of radiation by molecules. Energy levels in molecules. Born Oppenheimer approximation, Population of energy levels.

Optical Spectroscopy

Microwave spectroscopy: Molecular classification and Rotation spectra, Diatomic and polyatomic molecules. Application of Rotation spectra (Bond length, Isotopic mass, dipole moment, isotopic abundance), Non-rigidity of rotor.

Vibrational spectroscopy**:** Vibrational spectra of diatomics & SHO; anharmonicity & Morse potential; Vibration-rotational spectra of diatomics, polyatomic molecules-P,Q,R branches, Dispersive IR & FTIR, Vibration spectra of polyatomic molecules. Normal modes of vibrations of polyatomic molecules, Coupling of rotation and vibration, Parallel and perpendicular bands, Breakdown of Born-Oppenheimer Approximation,

Raman Spectroscopy: Polarizability and classical theory of Raman spectrum, Rotational Raman spectra. Vibrational Raman spectra, mutual exclusion principle, Surface enhanced Raman spectra, Resonance Raman,

Electron Spectroscopy: Electronic energy states of molecules. Vibrational structure of electronic bands, Electronic transitions and absorption bands, Selection rules, Electron spectroscopy for chemical analysis (ESCA)-UPS, X-ray photoelectron spectroscopy (XPS), Auger electron spectroscopy (AES).

Reference Books:

1. I. N. Levine: Quantum Chemistry, Prentice Hall India, 1994.
2. S. N. Datta: Lecture on Chemical bonding and quantum chemistry, 1998.
3. D. A. McQuairrie: Quantum Chemistry, Oxford University press, Oxford,1982.
4. P. W Atkins: Molecular Quantum Mechanics, Clarendon Press, Oxford, 1983.
5. R. K. Prasad: Quantum Chemistry through Problems and Solutions, New Age International, 1997.
6. F. L. Pilar: Elementary quantum chemistry, Mc-Graw Hill International, 2nd ed. 1990.
7. A. K Chandra: Introduction to Quantum Chemistry, Tata McGraw Hill, 1988.P. W. Atkins, Physical Chemistry, Oxford, London, *6th edi*, 1998.
8. R. Sindhu, Molecular Spectroscopy, Tata McGraw Hill, 1986.
9. Banwell, Molecular Spectroscopy, Tata McGraw Hill, 1998.
10. I. N. Levine: Quantum Chemistry, Prentice Hall India, 1994.
11. S. N. Datta: Lecture on Chemical bonding and quantum chemistry, 1998.
12. D. A. McQuairrie: Quantum Chemistry, Oxford University press, Oxford,1982.
13. P. W Atkins: Molecular Quantum Mechanics, Clarendon Press, Oxford, 1983.
14. R. K. Prasad: Quantum Chemistry through Problems and Solutions, New Age International, 1997.
15. F. L. Pilar: Elementary quantum chemistry, Mc-Graw Hill International, 2nd ed. 1990.
16. A. K Chandra: Introduction to Quantum Chemistry, Tata McGraw Hill, 1988.P. W. Atkins, Physical Chemistry, Oxford, London, *6th edi*, 1998.
17. R. Sindhu, Molecular Spectroscopy, Tata McGraw Hill, 1986.
18. Banwell, Molecular Spectroscopy, Tata McGraw Hill, 1998.
19. Graebeal, Molecular Spectroscopy, Prientice Hall, 1968.
20. G. M. Barrow, Introduction to Molecular Spectroscopy, McGraw Hill, 1964.

Semester VIII

Physical Methods in Chemistry I

Credits 4 **Theory**

Specific objectives:

To introduce the concepts of different spectroscopic techniques and its application in solving the structures of organic and inorganic compounds.

Learning outcomes:

Ensures the students to understand, acquire knowledge on advanced concepts in spectroscopy and thereby structure elucidation of unknown organic and inorganic compounds.

Electronic Spectroscopic: Basics of UV Spectroscopy, Applications to Organic Molecules, type of transitions, effect of solvent and substituents, Woodward Fieser rule and applications to polyenes, aromatic compounds and carbonyl compounds

Infra-Red Spectroscopy: Principle, instrumentation and sampling techniques, types of stretching and bending vibration – Factors influencing the vibrational frequency, vibrational frequencies of alkane, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenol, carbonyl compounds, amines and heterocyclics– related problems.

NMR Spectroscopy: ^{1}H NMR, Spectral parameters – intensity, chemical shift, multiplicity, coupling constant, factors affecting chemical shift. Analysis of first order and second - order spectra – shift reagents - structure determination of organic compounds by ^{1}H NMR spectra. Chemical shifts and coupling constants (spin-spin coupling) involving different nuclei (^{1}H,^{13}C) interpretation and applications to inorganic compounds. Examples for different spin systems – chemical shifts and coupling constants (spin-spin coupling) involving different nuclei (^{1}H, ^{19}F, ^{31}P, ^{13}C) interpretation and applications to inorganic compounds – Effect of quadrupolar nuclei (^{2}H, ^{10}B, ^{11}B) on the ^{1}H NMR spectra, Satellite spectra.
Systems with chemical exchange - evaluation of thermodynamic parameters in simple systems – study of fluxional behavior of molecules – an elementary treatment of second order spectra – examples – NMR of paramagnetic molecules – isotropic shifts contact and pseudo-contact interactions – Lanthanide shift reagents

^{13}C NMR: Proton coupled; off–resonance decoupled; proton noise decoupled ^{13}C NMR spectra. Assignment of chemical shifts, additively effect, characteristic chemical shifts of common organic compounds and functional groups, APT, DEPT and INEPT spectra. NMR of common heteroatoms present in organic compounds - 2D NMR techniques ^{1}H – ^{1}H COSY, ^{1}H – ^{13}C COSY – HMBC, NOESY and INADEQUATE.

Mass spectrometry: Elementary idea about mass spectrometry, interpretation of data and solving problems with spectrometric techniques, mass spectra of inorganic and organic molecules

***Microscopic Techniques*:** Principles of SEM, AFM, TEM and STM

Prescribed books

1. Silverstein, R. M., and Webster, F. X., Spectrometric identification of organic compounds, John Wiley and Sons. Inc., 6th edition, **1997**.
2. W. Kemp, Organic Spectroscopy, 3rd edition, MacMillon, **1994**.
3. Jag Mohan, Organic Spectroscopy: Principles & Applications, Narosa Publishers, **2012**.
4. Drago, R. S., *Physical Methods for Chemistry*, 2nd Edition, Saunders College Publishing, **1992**.
5. Lever, A. B. P., *Inorganic Electronic Spectroscopy*, 2nd Sub. Edition, Elsevier Science, **1986**.

Reference Books

1. Pavia, Lampman and Kriz, Introduction to Spectroscopy, Brooks/Cole Pubs Co, 5th edition, **2015**.
2. Williams, D. H., and Ian Fleming, Spectroscopic methods in organic chemistry, Tata McGraw Hill, **1998**.
3. William Kemp, NMR in chemistry: A multinuclear introduction, MacMillan, **1988**.
4. Organic Spectroscopy by L. D. S. Yadav, Kulwer academic publishers, **2004**.

5. Gerson, F., and Huber, W., Electron Spin Resonance Spectroscopy for Organic Radicals, Wiley-VCH, 1st edition, **2001**.
6. Cotton, F. A., and Wilkinson, G., *Advanced Inorganic Chemistry*, 3rd edition, Wiley-Eastern Company, New Delhi, **1990**.
7. J. AND Wilkins Lewis, R. G., *Modern Coordination Chemistry Principles and Methods*, Interscience Publishers, Inc., **1967**.
8. Ebsworth, E. A. V., Structural Methods in Inorganic Chemistry, 3rd edition, ELBS, Great Britain, **1987**.
9. Scott, R. A., and Lukehart, C. M., Applications of Physical Methods to Inorganic and Bioinorganic Chemistry, John and Wiley & Sons, LTD, **2007**.
10. Solomon, E. I., Lever, A. B. P., Inorganic Electronic Structure and Spectroscopy, Vol., 2, Applications and Case Studies, Wiley-Interscience, **2006**.
11. Satyanarayana, D. N., Electronic Absorption Spectroscopy, Universities Press, **2000**.
12. Jordon, R. B., Reaction Mechanisms of Inorganic and Organometallic Systems, 3rd edition, Oxford University Press, **2007**.
13. Ballhausen, C. J., and Gray, H. B., Molecular Orbital Theory, Benjamin/Cummings Pub. Co, **1965**.
14. Figgis, B. N., and Hitchman, M. A., *Ligand Field Theory and Its Applications*, 1st edition, Wiley VCH, **1999**.
15. Huheey, J. E., Keiter, E. A. and Keiter, R. L., and Medhi, O. K., *Inorganic Chemistry - Principles of Structure and Reactivity*,4th Edition, Pearson Education, **2006**.
16. Purcell, K. F. and Kotz, J. C., *Inorganic Chemistry*, Cengage Learning, **2012**.
17. A Carrington and A. D. Mclachlan, Introduction to Magnetic Resonance, Harper & Row, New York, 1979.
18. A. Carrington and Machlachlon, Magnetic Resonance, Harper & Row, 1967.
19. A Derome, Modern NMR Technique, Pergamon, 1983.
20. Farrar and E. D. Becker, Pulsed FT NMR Spectroscopy.
21. Wertz and Bolton, Electron Spin Resonance, McGraw Hill.
22. A. E. Derome, Modern NMR Techniques for Chemistry Research, Pregamon, 1987.
23. C. P. Slichter, Principles of Magnetic Resonance, Third Edition, Springer-Verlag, 1990.
24. T. C. Farrar and E. D. Becker, Pulse and Fourier Transform NMR, Academic Press, New York, 1971.

Semester VIII
Advanced Physical Chemistry Laboratory I

Credit: 4 **Practical**

Course objective

- To know the wet lab chemistry and computational chemistry practical experiments.
- To understand the concept chemical reactions in Kinetics, spectroscopy, surface chemistry, conductometry, potentiometry, viscometry etc.
- To perform Phase diagram with two component and three component systems.
- To know the redox process and determine the cyclic voltammetry method.
- To prove the computational calculate using electrostatic charges, resonance energy, dimerization energy, Gibbs free energy, pKa of the molecules, Docking studies etc.

Course outcome

After successful completion of this course, the students will able

- To enrich the knowledge about experiments in lab work and in computational work.
- To identify the concentration, adsorption isotherms, surface area, molecular formula, partition coefficient, stability constant, order of rate constant using the chemical compounds.
- To model novel organic/inorganic compounds in their ground state electronic configuration using computational methods.
- To evaluate and study the energy, concentration, structures and kinetics using various spectroscopic methods.

Part A: List of Wet Lab Chemistry

(Any 10-12 Experiments)

1. *Surface Chemistry*

a) Verification of adsorption isotherms (Freundlich and Langmuir): charcoal-acetic acid or charcoal-oxalic acid system.

b) Kinetics & Determination of surface area by adsorption of acetic acid on Charcoal

2. *Phase Diagram*

a) Determination of the concentration of the electrolyte using CST of phenol-water system

b) Three Component Liquid Systems: Acetic Acid – Chloroform – Water

3. *Partition Coefficient*

a) Partition coefficient of benzoic acid between benzene and water.

b) Molecular formula of copper-ammonia complex by the partition coefficient method

4. *Spectroscopy*

a) Formation kinetics of Chromium-EDTA complex (Spectrometry)

b) Simultaneous Estimation of Manganese and Chromium in a Solution of Dichromate and Permanganate Mixture

c) Photocalorimetric determination of Bimolecular rate constant

5. *Surface Tension*

a) Determine the surface excess of amyl alcohol.

6. *Potentiometry*

a) Titration of a strong and weak Acid Mixture with a Strong Base-Potentiometry

b) Determination of stability constant of silver diammine complex by potentiometric titrations

c) Dissociation of a weak acid by potentiometric titration

7. *Conductometry*

a) Verification of Ostwald's dilution law and determination of dissociation constant of weak acid

b) Conductometric titrations of a mixture of acids Vs strong base

c) Van't Hoff's factor of benzoic acid between benzene and water

d) Critical Micelle concentration of surfactant by conductivity measurements

e) Verification of Onsager's Equation and Determination of Equivalent Conductance at Infinite Dilution of Strong Electrolytes

f) Conductometric determination of Nickel using DMG

8. *Kinetics*

a) Second order rate constant for the alkaline hydrolysis of ethyl acetate by conductivity measurements

b) Arrhenius parameters for the Acid–Catalysed Hydrolysis of Methyl acetate

9. *Viscometry*

a) Determination of molecular weight of a polymer by viscosity measurements

10. *Additional*

a) Specific and molar refraction of a liquid by Refractometry

b) Reversibility of a redox process and determination of concentration of a given solution by cyclic voltammetry

c) Inversion of Sucrose-Polarimeter

Part B: List of Computational Chemistry Experiments

(Any 3-4 Experiments)

1. Calculation of electrostatic charges of atoms in organic molecules using population analysis
2. Calculation of Resonance energy of aromatic compounds
3. Calculation of dimerization energy of carboxylic acids
4. Perform the conformational analysis of butane using potential energy scan
5. Find the transition state of simple organic reactions and plot the reaction profile.
6. Determination of heat of hydration of organic molecules.
7. Find the Gibbs free energy of simple gaseous phase reactions and calculate equilibrium constant.
8. Calculation of pKa of simple organic molecules and compare it with experimental values
9. Docking studies involving protein ligand interactions.
10. Calculation of electrophilicity index in hard-soft acids and bases.

Reference Books

1. J.B. Yadav, Advanced Practical Physical Chemistry, Goel Publishing House, 2001.
2. G.W. Garland, J.W. Nibler, D.P. Shoemaker, Experiments in Physical Chemistry, 8th Edn. McGraw Hill, 2009.
3. B. Viswanathan, Practical Physical chemistry, Viva Pub., 2005
4. Saroj Kumar and Naba Kumar, Physical Chemistry Practical, New Central Book Agency,2012
5. Practical Physical Chemistry Paperback, 1974 by A.M. James, F.E. Prichard.
6. J. Foresman & Aelieen Frisch, Exploring Chemistry with Electronic Structure Methods, Gaussian Inc., 2000.
7. D.C. Young, Computational Chemistry: A Practical Guide for Applying Techniques to Real World Problems, John Wiley & Sons, 2001.
8. D. Rogers Computational Chemistry Using the PC, 3rd Edition, John Wiley & Sons (2003).
9. Leach, Molecular Modelling: Principles and Applications, 2nd Edn, Longman, 2001.
10. J. M. Haile (2001) Molecular Dynamics Simulation: Elementary Methods.

Semester IX
Physical Methods in Chemistry II

Credit: 4 **Theory**

Specific objectives:

To introduce spectroscopic techniques to solve structure of metal complexes.

Learning outcomes:

Ensures the students to understand, acquire knowledge on advanced concepts in spectroscopy thereby able to solve spectrum to structure of metal complexes.

Electronic Spectroscopy: Microstates, - terms and energy levels for d^1 - d^9 ions in cubic and square fields – Intensity of bands – group theoretical approach to selection rules - Effect of distortion and spin-orbit coupling on spectra- Orgel and Tanabe-Sugano diagrams – Evaluation of 10Dq and β for octahedral complexes of cobalt and nickel – applications to simple coordination compounds – charge transfer spectra – electronic spectra of $[Ru(bipy)_3]^{2+}$. Electronic Spectra of f-block elements.

Optical rotatory dispersion, circular dichroism and Magnetic circular dichroism – applications to metal complexes. Basic principles of inorganic photochemistry.

***Infrared and Raman Spectroscopy*:** Group vibrations and the limitations- combined uses of IR and Raman Spectroscopy in the structural elucidation of simple molecules like N_2O, ClF_3, NO_3^-, ClO_4^- effect of coordination on ligand vibrations – uses of groups vibrations in the structural elucidation of metal complexes of urea, thiourea, cyanide, thiocyanate, nitrate, sulphate and dimethyl sulfoxide – Effect of isotopic substitution on the vibrational spectra of molecules – vibrational spectra of metal carbonyls with reference to the nature of bonding, geometry and number of C-O stretching vibrations (group theoretical treatment) – Applications of Raman Spectroscopy – Resonance Raman Spectroscopy.

EPR spectroscopy: Theory of EPR spectroscopy - Spin densities and McConnell relationship – Factors affecting the magnitude of g and A tensors in metal species - Zero-field splitting and Kramers degeneracy – Spectra of VO(II), Mn(II), Fe(II), Co(II), Ni(II) and Cu(II) complexes – Applications of EPR to a few biological molecules containing Cu(II) and Fe(III) ions. Magnetic properties -Determination of Magnetic moments and their applications to the elucidation of structures of inorganic compounds – temperature independent paramagnetism. Magnetic properties of lanthanides and actinides. Spin crossover in coordination compounds – Single molecule magnets.

Mössbauer Spectroscopy: Isomer shifts – Magnetic interactions – Mossbauer emission spectroscopy – applications to iron and tin compounds.

NQR spectroscopy: Characteristics of quadrupolar nucleus – effects of field gradient and magnetic field upon quadrupolar energy levels – NQR transitions – applications of NQR spectroscopy.

Prescribed Books:

1. R. S. Drago, *Physical Methods in Inorganic Chemistry*, Van Nostrand Reinhold Inc., U. S., 1965.
2. R. S. Drago, *Physical Methods for Chemistry*, 2nd Edition, Saunders College Publishing, 1992.
3. A. B. P. Lever, *Inorganic Electronic Spectroscopy*, 2nd Sub Edition, Elsevier Science, 1986.
4. J. E. Huheey, E. A. Keiter and R. L. Keiter and O. K. Medhi, *Inorganic Chemistry –Principles of Structure and Reactivity*, 4th Edition, Pearson Education, 2006.
5. A. K. Das and M. Das, *Fundamental concepts of Inorganic Chemistry,* 1st Edition, Volume 7, CBS Publishers & Distributors Pvt Ltd. 2014.
6. Wulfberg, G., *Inorganic Chemistry*, University Science Books, 2000.
7. K. Nakamoto, Infrared and Raman Spectra of Inorganic and Coordination Compounds, Part B: Applications in Coordination, Organometallic, and Bioinorganic Chemistry, Wiley-Interscience; 5th edition, 1997.
8. J. Ferraudi, Elements of Inorganic Photochemistry, Wiley, New York, 1988.

Reference Books

1. F. A. Cotton and G. Wilkinson,*Advanced Inorganic Chemistry*, 3rd ed., Wiley-Eastern Company, New Delhi, 1990.
2. P. J. Wheatley, *The Determination of Molecular Structure*, 2nd Edition, Dover Pubns, 1981.
3. J. AND R. G. Wilkins Lewis, *Modern Coordination Chemistry Principles and Methods*, Interscience Publishers, Inc., 1967.
4. E. A. V. Ebsworth, Structural Methods in Inorganic Chemistry, 3rd ed., ELBS, Great Britain, 1987.
5. R. A. Scott and C. M. Lukehart, Applications of Physical Methods to Inorganic and
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7. E. I. Solomon, A. B. P. Lever, Inorganic Electronic Structure and Spectroscopy, Vol.,2 Applications and Case Studies, Wiley-Interscience, 2006.
8. B. P. Lever, Inorganic Electronic Spectroscopy, 2nd Sub Edition, Elsevier Science, 1986.
9. D.N. Satyanarayana, Electronic Absorption Spectroscopy, Universities Press, 2000.
10. R.B. Jordon, Reaction Mechanisms of Inorganic and Organometallic Systems, 3rd Edition, Oxford University Press, 2007.
11. C.J. Ballhausen and H.B. Gray, Molecular Orbital Theory, Benjamin/Cummings Pub. Co, 1965.
12. N. Figgis and M. A. Hitchman, *Ligand Field Theory and Its Applications*, 1st Edition, Wiley VCH, 1999.
13. A.W.Adamson, Inorganic Photochemistry, John Wiley & Sons, New York.
14. S.F.A. Kettle, Physical Inorganic Chemistry – A Coordination Chemistry Approach,
15. Spectrum Academic Publishers, Oxford University Press, 1996.
16. W. Adamson and P. D. Fleischauer, Concepts of Inorganic Photochemistry, Wiley, New York, 1975.

Semester IX
Reagents & Synthetic Strategies in Organic Chemistry

Credit: 4 **Theory**

Specific objectives:
To introduce the advanced synthetic methodologies involving modern synthetic reagents, protecting groups and planning organic synthesis.

Learning outcomes:
Ensures the students to understand, acquire knowledge on modern synthetic reagents, protecting groups and planning of organic synthesis through disconnection approach.

Protecting and Deprotecting Strategies: Need for protection and deprotection of functional groups during chemical reactions- protection of hydroxyl, mercapto, amino, carbonyl and carboxylic groups.

Planning Organic Synthesis: An introduction to reterosynthesis - Synthon – synthetic equivalent – target molecule, functional group interconversion. Disconnection approach- one group disconnection- disconnection of alcohols, olefins and ketones. Logical and illogical disconnections. Two group disconnection-1,2, -1,3, 1,4, 1,5 and -1,6 dioxygenated skeletons and dicarbonyls; Umpolung, antithesis, chiron. C-C bond forming reactions (alkylation as well as enamine alkylation). Retro Diels – Alder reactions- Pericyclic reactions- Reterosynthesis of heterocycles containing two nitrogens. Designing synthesis: Disconnection approach in Camphor, reserpine and longifolence,

Synthetic Reagents: Use of the following reagents in organic synthesis and functional group transformations: Sodium borohydride, tri-n-butyl tin hydride, lithium dimethyl cuprate, lithium diisopropyl amide, trimethyl silyl iodide, diborane, ozone, CrO_3 DCC, DDQ, 9-

BBN, lead tetra acetate, phenyl iodoso acetate, dimethyl sulphoxide, SeO_2, PCC, Yeast. Phase transfer catalysis – benzyltriethylammonium halides- crown ethers.

Functional group transformations using reducing reagents: Use of $NaBH_4$, $NaCNBH_3$, $LiAlH_4$ and Bu_3SnH; Use of Sn/HCl, Zn/HCl, Hydrazine, Li-NH_3, Na/alcohol, Pd/H_2 and Raney Ni.

Prescribed books

1. Smith M. B.,March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 7th edn, Wiley, **2015**
2. Carey, F.A., Sundberg, R.J., Advanced Organic Chemistry, Part A: Structure and Mechanisms, 5th edn, Springer, **2007.**
3. Carey, F.A., Sundberg, R.J., Advanced Organic Chemistry, Part B: Reaction and Synthesis, 5th edn, Springer, **2007.**
4. Clayden,J.,Greeves,N.,Warren.S.Organic Chemistry,2ndedn,Oxford University Press, **2014**
5. Li, J. J., Corey, E. J., Name Reactions for Homologation, Part 1, Wiley-Blackwell, **2009**
6. Mundy, B. P., Ellerd, M G., Favaloro Jr. F. G., Name Reactions and Reagents in Organic Synthesis, 2nd edn, Wiley-Blackwell, **2005**
7. Carruthers, W., Coldham, I., Modern Methods of Organic Synthesis, 4th edn, Cambridge University Press, **2015**
8. Norman, R. O. C., Coxon, J. M., Principles of Organic Synthesis, 3rd edn, **1993.**
9. Wyatt, P., Warren, S., Organic Synthesis: Strategy and Control, Wiley-Blackwell, **2007**
10. Warren, S., Wyatt, P., Organic Synthesis: The Disconnection Approach, Wiley, **2008**
11. Corey, E. J., Cheng, X. M. The Logic of Chemical Synthesis, Wiley-India Private Ltd, **2011**
12. Nicolaou, K. C., Sorensen, E. J., Classics in Total Synthesis, Wiley-ECH**, 1996**

Semester IX
Thermodynamics (Classical & Statistical) & Electrochemistry

Credit: 4 **Theory**

Course objective:

- To know the concepts of classical as well as statistical Thermodynamics
- To study about the Basic and essential of electrochemistry in distinct phenomena (in Equilibrium and Dynamic).
- To understand the tuned concept of electrochemistry in storage cells.
- To aware about the recent applications using the concepts of electroanalytical techniques.

Course outcome:

After successful completion of this course, the students will able

- To enrich the knowledge about the basic laws of thermodynamics and fundamentals of statistical thermodynamics.
- To observe the electrochemical ideas at equilibrium and dynamics progress.
- To familiar in storage cells concepts using the principle of electrochemistry.

Classical Thermodynamics

Introduction: Laws of thermodynamics, Entropy- Free Energy-Systems of Variable Compositions - Fugacity and Activity Maxwell's relations – significance, Partial molar properties – Chemical potential, Fugacity and Activity. Concept of absolute entropy and residual entropy

Thermodynamics of mixing: Thermodynamic functions of mixing, Clausius Inequality, Gibbs-Duhem-Margules equation, Konowaloff's rule, Henry's law, excess thermodynamic functions

Chemical Equilibrium: Chemical affinity and thermodynamic functions, effect of temperature and pressure on chemical equilibrium- van't Hoff equations.

Third law of thermodynamics: Nernst heat theorem, development of third law of thermodynamics, determination of absolute entropies using third law, entropy changes in chemical reactions.

Thermodynamics of Irreversible Processes: Thermodynamics of irreversible processes with simple examples. phenomenological relations. Onsager reciprocal relations - principle of microscopic reversibility. Electrokinetic phenomena. Thermoelectric phenomena.

Statistical Thermodynamics

Fundamentals of Statistical Thermodynamics: Thermodynamic probability, Stirlings approximation microstate and macrostate, entropy and probability, most probable distribution, Maxwell - Boltzman statistics. Distribution Law-Effect of temperature on distribution, Calculation of most probable velocity, average and mean square velocity, components of velocity, Mean free path, Effusion and diffusion, thermal conductivity and viscosity of gases. Heat capacity of gases - classical and quantum theories, heat capacity of hydrogen

Partition and Thermodynamic Functions: Partition function and its relation to thermodynamic properties, Translational, rotational and Vibrational partition function. Heat

capacity of solids: Dulong - Petits law, Einstein's theory and its modification, Debye's theory of heat capacity of solids.

Quantum statistics: Bose - Einstein statistics & distribution, example of particles, Bose-Einstein condensation, difference between first order and higher order phase transitions, liquid helium, supercooled liquids. Fermi - Dirac statistics, Fermi-Dirac distribution: examples of particles, application in electron gas, thermionic emission. Comparison of three statistics

Electrochemistry

Activity and Activity coefficient of electrolytes, ionic strength, Debye Huckel theory of strong electrolytes, Debye Huckel limiting law, Mean ionic activity coefficient. Application of Debye Huckel theory to - Relaxation and electrophoretic effects, Debye-Huckel-Onsager equation and its derivation. Debye Falkenhagen effect. Wein effect. Ionic activity coefficients of strong electrolytes- Derivation of Debye-Huckel limiting law.

Equilibrium Electrochemistry: EMF Phenomena, Cell Potential and its measurement, reference electrodes. Electrochemical cells, concentration cells and activity coefficient determination, liquid junction potential, Determination of solubility. pH Conductometric, Potentiometric and pH titrations, Redox indicators and redox titrations.

Dynamic Electrochemistry: Electrical double layer, various models of electrical double layer, Electrode polarization. Overpotential, hydrogen and oxygen overvoltage, theories of overvoltage, Butler-Volmer equation for simple electron transfer reactions, Tafel plot and its significance, Corrosion: stability of metals, Porbaus diagram-Evan diagram-corrosion control and methods for prevention.

Storage cells: Lead acid battery, Lithium battery, nickel cadmium cell. Fuel Cell. Theory and working of fuel cell. H_2- O_2 fuel cell, methanol fuel cell, Solid oxide fuel cells.

Electroanalytical Techniques**:** Polarography – diffusion current, supporting electrolyte, three electrode system, polarographic maxima. Amperometry – principles and applications – Types of amperometry. Cyclic voltammetry – principles, applications. Stripping voltammetry.

Reference Books:

1. R.P. Rastogi, R.R. Mishra, An introduction to Chemical Thermodynamics, Vikas publishing house, **2009.**
2. J. Rajaram, J.C. Kuriakose, Thermodynamics, S Chand and Co**., 1999**.
3. M.C. Gupta, Statistical Thermodynamics, New age international, **2007**.
4. L.K. Nash, Elements of Classical and Statistical Mechanics, 2nd Edn. Addison Wesley, **1972.**
5. F.W. Sears, G.L. Salinger, Thermodynamics, Kinetic Theory and Statistical Thermodynamics, Addison Wesley, **1975.**
6. J. Kestin, J.R. Dorfman, A Course in Statistical Thermodynamics, Academic Press, **1971**
7. John E. Freund. Modern elementary statistics**, 2003**, ISBN-13: 978-0131874398 20.
8. S. P. Gupta, Statistical Methods: S. Chand, **2014.**
9. J. Bockris and A.K.N. Reddy, Modern Electrochemistry, 2B, 2nd Edn., Wiley, New York, **1998**
10. D.R. Crow, Principles and Applications of Electrochemistry, Chapman & Hall, 3rd Edn., New York, **1994**

11. S. Glasstone, Introduction to Electrochemistry, Biblio Bazar, **2011.**
12. B.K. Sharma, Electrochemistry, Krishna Prakashan, **1985.**
13. A.I. Vogel, A Textbook of Quantitative Analysis including Instrumental Analysis, John Wiley & Sons, **1961.**
14. H.H. Willard, J. A. Dean, L.L. Merritt, Instrumental Methods of Analysis, Van Nostrand**, 1965.**
15. D.A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, Fundamentals of Analytical Chemistry, 8th Edn. Saunders College Pub., **2007.**

Semester IX
Advanced Inorganic Chemistry Laboratory

Credit: 4 **Practical**

Specific objectives:
To introduce multistep inorganic compound synthesis and purification, separation and spectroscopic analysis. Estimation of metal ions by spectrophotometry.

Learning outcomes:
Ensures the students to understand, acquire knowledge and have hands on experience in multistep inorganic compound synthesis and analysis by using spectroscopic techniques, Separation techniques.

Preparation of the following compounds and their Characterization

1. Tetramminecopper(II) sulphate.
2. Potassium trioxalatochromate(III).
3. Potassium trioxalatoaluminate(III).
4. Trithioureacopper(I) chloride.
5. Dibenzyltin dichloride.
6. Nitro and nitrito linkage isomers
7. Mn_3 clusters

1. Synthesis and study of Tris(oxalato)iron(III) potassium salt by Cyclic Voltammetry (CV) and Differential Pulse Voltammetry (DPV), and determination of the following: the formal reduction potential (E_o'); the number of electrons transferred in the redox process (n); electrochemical reversibility.
2. Synthesis and study of Mn^{III}(Salen)Cl by Cyclic Voltammetry and Differential Pulse Voltammetry (DPV), and determination of the following: the formal reduction potential (E_o'); the number of electrons transferred in the redox process (n); electrochemical reversibility.
4. Preparation and determination of the effective magnetic moment and number of unpaired electrons in $Mn(acac)_3$.
5. Preparation and determination of the aquation rate of $[Co(NH_3)_5Cl]Cl_2$.
6. Preparation and resolution of the optically active compound $[Co(en)_3]^{3+}$.
7. Preparation and characterization of (Mesitylene)tricarbonylmolybdenum(0) by solution infrared spectrum.
8. Bioanalytical techniques – Monitoring the cleavage of DNA and protein by metal complexes using Gel electrophoresis techniques – Agarose and PAGE (Demo only).

Reference Books

1. Elias, A. J., A Collection of Interesting General Chemistry Experiments, Universities Press, Sangam Books Ltd, **2002**.
2. Woollins, J. D., Inorganic experiments, 3rd edition, Wiley-VCH Verlag GmbH @ Co. KGaA, **2012**.
3. Hein, M., Peisen, J. N., and Miner, R. L., Foundations of College Chemistry in the Laboratory, John Wiley and Sons, **2011**.
4. Girolami, G. S., Rauchfuss,T. B., and Angelici, R. J., Synthesis and Technique in Inorganic Chemistry: A Laboratory Manual, 3rd edition, University Science Books, **1999**.
5. Jolly, W. L., The Synthesis and Characterization of Inorganic Compounds, Prentice-Hall, Inc.**1970**.
6. In-house Laboratory Manual, Department of Chemistry, CUTN.
7. Ghoshal, Mahapatra and Nad, An Advanced Course in Practical Chemistry, New Central Book Agency, **2011**.

Semester X
Project

Credit: 12 **Practical**

List of Electives

Course Code	Title of the Course	Credits
CYE001	Principles of Polymer Science	4
CYE002	Principles of Fluorescence Spectroscopy	4
CYE003	Asymmetric Catalysis	4
CYE004	Essentials of Carbohydrate Chemistry	4
CYE005	Organic Electronics	4
CYE006	Photochemistry in Molecules and Materials	4
CYE007	Medicinal Inorganic Chemistry	4
CYE008	Organic Semiconductors	4
CYE009	Advances in Polymer Science	4
CYE010	Advances in Carbohydrate Research	4
CYE011	Advanced Organic Materials and Catalysis	4
CYE012	Chemistry of CH Activation	4
CYE013	Advanced Bio-inorganic Chemistry	4
CYE014	Principles of Biochemistry	4
CYE015	Mathematics for Chemists and biologists	4
CYE016	Electrochemical Energy Systems	4
CYE017	Fundamentals of Analytical Chemistry	4
CYE018	Computational Chemistry	4
CYE019	Supramolecular Chemistry	4
CYE020	Mathematical methods in Chemistry	4

CYE021	Organometallics, Catalysis and Inorganic Spectroscopy	4
CYE022	Physical methods in Chemistry	4
CYE023	Applications of Computational Methods in Chemistry	4
CHEE24	Chemical Lab Safety and Management	4
CHEE25	Advances in Organic Chemistry	4
CHEE26	Green Chemistry	4
CHEE27	Selected topics in synthetic organic Methods	4
CHEE28	Advanced Topics in Organometallic Chemistry	4
CHEE29	Industrial Chemistry	3
CHEE30	Advanced Organic Nanomaterials	4
CHEE31	Computer software for Chemists	2
CHEE32		2

* New electives will be appended based on the availability of course instructor. Electives will be offered based on the individual faculties availability