

CENTRAL UNIVERSITY OF TAMIL NADU

Thiruvarur



Department of Chemistry
Integrated M.Sc (iM.Sc) Chemistry Syllabus

Name of the course	:	Integrated M. Sc. (Chemistry)
Duration	:	10 semesters
Intake	:	30
Eligibility	:	Plus two examination or equivalent of any recognized board in India with 60% marks (Chemistry, Mathematics, Physics and Computer Science/Biology) for general category, 55% for OBC (Non-creamy layer) and 50% for SC/ST candidates. The candidates should not have completed 20 years of age as on 01-07-2014.

Course Structure

The first two years of the integrated M.Sc (iM.Sc) Chemistry programme is balanced with foundation courses like language, eco-criticism, social studies, etc., and courses of chemistry, physics, mathematics, life science. 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. An open-ended lab in the fourth year followed by a dedicated research project that yields a dissertation report as part of the curriculum brings out the best in our students, which will motivate in pursuing research career.

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

Semester	Course Code	Course Title	Number of Credits
1	CHE0101	General Chemistry I	3
2	CHE0201	General Chemistry II	3
	CHE0202	General Chemistry Practical I	2
3	CHE0301	General Chemistry III	3
	CHE0302	General Chemistry Practical II	2
4	CHE0401	General Chemistry IV	3
	CHE0402	General Chemistry Practical III	2
5	CHE0501	Inorganic Chemistry I	4
	CHE0502	Structure and reaction mechanisms	4
	CHE0503	Kinetics, Surfaces and Interfaces	4
	CHE0504	Analytical Chemistry - Instrumental methods of analysis	4
	CHE0505	Inorganic and Analytical Chemistry Techniques	3
	CHE0506	Organic Chemistry Laboratory I	3
6	CHE0601	Inorganic Chemistry II	4
	CHE0602	Reaction mechanisms and organic photochemistry	4
	CHE0603	Introductory Quantum Chemistry	4
	CHE0604	Solutions and Soft Matter	4
	CHE0605	Physical Chemistry Practical I	3
	CHE0606	Organic Chemistry Practical II	3
7	CHE0701	Inorganic Chemistry III	4
	CHE0702	Reaction mechanism, reagents and reactivity	4
	CHE0703	Symmetry and Group Theory of Molecules	4
	CHE0704	Physical methods in organic chemistry	4
	CHE0705	Advanced Organic Synthesis Laboratory	3
	CHE0706	Physical Chemistry Laboratory II	3
8	CHE0801	Bioinorganic Chemistry and Inner-transition elements	4
	CHE0802	Organic reaction mechanisms	4
	CHE0803	Introduction to Molecular Spectroscopy	4
	CHE0804	Physical Methods in Inorganic Chemistry	4
	CHE0805	Advanced Inorganic Chemistry Laboratory	3
	CHE0806	Open ended Laboratory	3
9	CHE0901	Main-Group and Organometallic Chemistry	4
	CHE0902	Chemistry of Biopolymers and natural products	4
	CHE0903	Advanced Thermodynamics	4
	CHE0904	Advanced Organic Synthesis	4
	CHE0905	Computational Chemistry Laboratory	3
	CHE0906	Seminar and Literature Review	3
10	CHE1001	Research Project	9
	CHE10xx	Elective 1	3
	CHE10xx	Elective 2	3
	CHE10xx	Elective 3	3
	CHE10xx	Elective 4	3
TOTAL			149

CHE10xx - Electives

CHE0101

Semester: 1

Subject Code: CHE0101

Credits: 3

2-1-0-3

Title: General Chemistry I**Introduction:** Units, dimensions, Stoichiometry, concepts of mole**Electronic Structure and Periodic Properties:** Hydrogen atomic orbitals and their description. Quantum numbers – principal, azimuthal, magnetic and spin quantum numbers and their significance - radial and radial distribution functions-angular functions – principles governing the occupancy of electrons in various quantum levels – Pauli's exclusion principle – Aufbau principle – Hund's rule – (n+1) rule – stability of half-filled and fully-filled orbitals.

Periodic properties – variation of atomic volume, atomic and ionic radii, ionization potential, electron affinity and electronegativity along periods and groups – factors affecting the periodic properties.

Chemical Bonding: Ionic bond – lattice energy and Born-Haber cycle (no derivation) - Fajan's rules elementary crystal structures, fcc, bcc and simple cubic lattices. Covalent bond – hybridization, polarity of bonds – Ionic character of covalent bond and electronegativity- coordinate bond. Qualitative MO theory, Sigma, Pi and Delta bonds, Octet and EAN rules.VSEPR theory - shapes of simple inorganic molecules containing lone pairs and bond pairs of electrons (BeCl₂, NH₃, H₂O, PCl₃, XeF₄, SF₄, BrF₅, ClF₅, PCl₅, SF₆). Intermolecular forces – Non-covalent interaction, van der Waals forces and hydrogen bonding.**Introductory Organic Chemistry:** IUPAC nomenclature: Alkanes, cycloalkanes, alkenes, alkynes, halogen compounds, alcohols, ethers, aldehydes, ketones and carboxylic acids; Hybridization and Geometry of Molecules: methane, ethane, ethylene, acetylene; Electronic Effects: Inductive, resonance, hyperconjugation and steric effect; Cleavage of bonds: Homolytic and Heterolytic C-C bond fission; Reaction Intermediates and their stability: Carbocations, carbanions and free radicals.**Gaseous State:** Gas laws, Kinetic theory of gases**Nuclear Chemistry:** Basics of nuclear chemistry**Prescribed Books**

1. Whitten, K.W; Davis, R.E; Peck, L; Stanley, G.G; Chemistry, Cengage Learning; 9th edition, **2009**.
2. Chang, R.; Goldsby, K.; Chemistry, Mc-Graw Hill, 11th edition, **2012**.
3. Mahan, B. H.; Myers, R. J.; University Chemistry, Benjamin-Cummings Publishing Company; 4th Sub edition, **2000**.
4. Morrison, R. T.; Boyd, R. N.; Organic Chemistry, 6th edition, **2000**.
5. Lee, J.D.; *Concise Inorganic Chemistry*, Blackwell Science, 5th edition, **1996**.
6. Atkins, P. W.; Paula, J.; Physical Chemistry, Oxford Publications, 8th edition, **2009**.
7. Sharpe, A.G; *Inorganic Chemistry*, 3rd Edition, Pearson, **2010**.

Reference Books

1. Shriver, D.; Atkins, P. W.; Inorganic Chemistry, W.H.freeman and Company, 5th edition, **2009**.
2. Miessler, G. L.; Tarr, D. A.; Inorganic Chemistry, Prentice Hall, 4th edition, **2010**.
3. C. N. R. Rao, *Understanding Chemistry*, University Press (India) Ltd., 2001.

4. Castellan, G. W.; Physical Chemistry, Narosa Publishing House, 3rd edition, **2004**.
5. Raff, L. M.; Principles of Physical Chemistry, Prentice Hall, **2001**.
6. Shillady, D.; Essentials of Physical Chemistry, CRC Press, **2012**.
7. Huheey, J. E.; Keiter, E. A.; Keiter, R. L.; Inorganic Chemistry - Principles of Structure and Reactivity, Pearson Education, 4th edition, **2006**.
8. Douglas, B.; McDaniel, D.; Alexander, J.; Concepts and Models of Inorganic Chemistry, 3rd edition, John Wiley & Sons, **2010**.
9. Volhardt, K.P. C.; Schore, N. E.; Organic Chemistry, W. H. Freeman and Company, **1990**.
10. Pine, S. H.; Organic Chemistry, Tata McGraw Hill, 5th edition, **2008**.
11. Finar, I. L.; Organic Chemistry, Pearson education India, 6th edition, *vol-1*, **2011**.

Semester: 2**Subject Code: CHE0201****Credits: 3****2-1-0-3****Title: General Chemistry II**

Chemical Thermodynamics: Thermodynamic terminology, State and path functions. Concept of heat and work. First Law of thermodynamics, energy and enthalpy. Thermodynamic processes. Heat capacities. Calculation of w , q , dU & dH for the expansion of ideal gases under isothermal and adiabatic condition for reversible process.

Introduction to Thermo-chemistry, Kirchhoff's equation and applications: Entropy, entropy changes in reversible and irreversible processes, physical concept of entropy, entropy changes of an ideal gas in different processes, entropy of an ideal gas, Free energy concept, Gibbs and Helmholtz free energies, variation of free energy with temperature and pressure. Gibbs-Helmholtz equations, Criteria for reversible and irreversible processes based on entropy and free energy.

Equilibria: Chemical, Ionic and Phase: Introduction to equilibrium, equilibrium constants, Le Chatelier's principle, Chemical equilibrium; law of mass action; K_p , K_c and K_x ; van't Hoff equation; Acid Base and Ionic Equilibria - Arrhenius theory, Acids and bases in proton solvents, Bronsted-Lowery theory, Concepts of a strong, weak acids and bases; pH scale; Henderson-Hasselbach equations; Buffer solutions; Acid base indicators; solubility product.

Phase Equilibria - Phase, Components, Degree of freedom, Phase rule, one component system and two component system examples; Calculation of eutectic point, composition. Introduction to Nernst distribution law.

Electrochemistry: Arrhenius theory of electrolytic dissociation, classification of electrolytes Conductance concepts; Cell constant; Applications of conductance measurements: degree of dissociation of weak electrolytes, dissociation constant of weak acids, determination of solubility of sparingly soluble salts, degree of dissociation of water, conductometric titrations.

Galvanic cells, reversible and irreversible cells, cell emf and its measurement. Reactions in reversible cells, free energy and emf of reversible cell. Single electrode potential (Nernst equation), its measurement and sign convention. Standard electrode potential. Emf of reversible cell from electrode potentials. Types of reversible electrode, reference electrodes.

Applications of emf measurements: determination of ionic activities, pH, potentiometric titrations (acid-base, redox, precipitation type reactions), equilibrium constant.

Chemical Kinetics: Rate of reaction and rate laws; molecularity and order of reactions– Zero, first and second order reactions. Pseudo first order reactions; Introduction to collision theory of reaction rates – activation energy and the Arrhenius equation, elementary reaction, reaction mechanisms, catalysis.

Prescribed Books

1. Silbey, R. J.; Albert, R. A.; Bawendi, M. G.; Physical Chemistry, Wiley, 4th edition, **2004**.
2. R. Chang, Chemistry, 1st Indian Edition, Tata-McGraw Hill, **2007**.
3. Atkins, P. W.; Paula, J.; Physical Chemistry, Oxford Publications, 8th edition, **2009**.

Reference Books

1. Castellan, G. W.; Physical Chemistry, Narosa Publishing House, 3rd edition, **2004**.
2. Kapoor K. L.; Physical Chemistry: Thermodynamics, Macmillan Publishers India Ltd, **2004**.
3. Raff, L. M.; Principles of Physical Chemistry, Prentice Hall, **2001**.
4. Laidler, K. L.; Chemical Kinetics, Pearson Education Inc, 3rd edition, **2011**.
5. McQuarrie, D. A.; Simon, J. D.; Physical Chemistry: A Molecular Approach, University Science Books, **2011**.
6. Levine, I. N.; Physical Chemistry, McGraw-Hill Science/Engineering/Math, 6th edition, **2008**.
7. Shillady, D.; Essentials of Physical Chemistry, CRC Press, **2012**.

Semester: 2

Subject Code: CHE0202

Credits: 2

0-0-3-2

Title: General Chemistry Practical - I

Basics of Laboratory

1. Demonstration and concept of good lab practices including safety, glassware handling, chemical nature understanding, chemical handling, chemical/glassware waste management, Error Analysis, notebook maintenance.
2. Calibration and handling of balances, pipettes and burettes, basic principles & experiments related to sample & reagent preparation: practical concept of Molarity, Molality, Normality, equivalence, weight %, vol.%, Preparation of standard solutions, Dilution 0.1 M to 0.001 M solutions.

Volumetric Analysis

I. Acidimetry and Alkalimetry

1. Estimation of NaOH using standard Na_2CO_3 solution and link HCl solution
2. Estimation of HCl using standard H_2SO_4 solution and link NaOH solution

II. Permanganimetry

3. Estimation of FAS (Mohr's salt) using standard FeSO_4 solution and link KMnO_4 solution
4. Estimation of hydrogen peroxide using standard oxalic acid solution and link KMnO_4 solution

III. Iodo and Iodimetry

5. Estimation of copper by using standard $\text{K}_2\text{Cr}_2\text{O}_7$ solution and link Sodium thiosulphate solution

IV. Complexometric

6. Estimation of Zinc by using standard zinc sulphate solution and link EDTA solution

Qualitative Analysis

Semi-micro analysis of a mixture containing two anions and two cations. (Interfering anions)

Reference Books

1. Vogel's quantitative chemical analysis, GH Jeffery, J Bassett, J Mendham, R C Denney, 5th edition, Longman Scientific and Technical, **1989**.
2. G. Svehla: *Vogel's qualitative inorganic analysis*, 7th Edition, Prentice Hall, **1996**
3. J. Mendham, R. C. Denney, J. D. Barnes, M. J. K. Thomas: *Vogel's Prescribed book of qualitative chemical analysis*, 6th Edition, Prentice Hall, **2000**.
4. Foundations of College Chemistry in the Laboratory, Morris Hein, Judith N. Peisen and Robert L. Miner, John Wiley and Sons, **2011**
5. Woollins, J. D; *Inorganic experiments*, 3rd Edition, Wiley-VCH Verlag GmbH Co. KGaA, **2012**.
6. Rao, C. N. R. and Agarwal, U. C; *Experiments in General chemistry*, Affiliated East-West Press, **1969**

Semester: 3

Subject Code: CHE0301

Credits: 3

2-1-0-3

Title: General Chemistry III

Basic Organic Synthesis and Principles: Alkanes: preparation by reduction of alkyl halides, Wurtz reaction and Kolbe's electrolytic methods with mechanism; Alkenes: preparation by dehydration of alcohols, dehydrohalogenation of alkylhalides, dehalogenation of vicinal dihalides and by Kolbe's electrolytic method; Alkynes: Preparation by dehydrohalogenation of vic-dihalides and gem-dihalides, dehalogenation of tetrahalides and Kolbe's electrolytic method; Reactions: Mechanism of free radical halogenation of alkanes, Addition reactions with halogens, hydrogen halide (Markovnikov's rule, peroxide effect), hydroboration, ozonolysis, hydroxylation with KMnO_4 , allylic substitution by NBS; Types of dienes - conjugated Dienes: 1,3-Butadiene-preparation, stability- 1,2 & 1,4 - addition, Diels- Alder reaction.

Methods of determining reaction mechanism: Thermodynamic and kinetic requirements of a reaction – Hammond's postulate –principle of microscopic reversibility – kinetics Vs thermodynamic control –methods of determining mechanisms – identification of products – intermediates – catalysis – kinetic studies – stereo chemical outcome, detection and trapping of intermediates – crossover experiments.

Stereochemistry I: Introduction, Concept of Isomerism, Classification of Stereoisomers, Optical isomerism, Chirality & Elements of symmetry, Wedge formula, Fischer projection, Newman projection. Relative and absolute configurations, sequence rules, D & L, R & S systems of nomenclature. Understanding with examples for Enantiomers, meso form, diastereoisomers, inversion, retention, and racemization. Geometrical Isomerism: About C=C, E-Z notation-determination of configuration. Conformational Analysis: Ethane, 1,2 – dihalo and dihydroxyethanes and butane.

Heterocycles I: Nomenclature of Heterocyclic compounds - Molecular orbital picture and aromatic characteristics of pyrrole, furan, thiophene and pyridine. Comparison of basicity of pyridine, piperidine and pyrrole.

Prescribed books

1. R. T. Morrison, R. N. Boyd and S. K. Bhattacharjee, *Organic Chemistry*, Seventh Edition, Pearson Prentice Hall, **2011**.
2. I.L.Finar, *Organic Chemistry, Volume 1, 6th edition*, Pearson education India, **2011**.
3. F.A.Carey and R.J.Sundberg, *Advanced Organic Chemistry, Part A: Structure and Mechanisms*, 5th edition, **2007**.
4. D. Nasipuri, *Stereochemistry of Organic Compounds: Principles and Applications*, 4th edition, New Academic Science Publisher.
5. Ernest L Eliel, Samuel H. Wilen, *Streochemistry of organic compounds*, Wiley India Edition, **2008**.

Reference books

1. K. Peter, C. Vollhardt and N. E. Schore, *Organic Chemistry*, W. H. Freeman and Company, **2010**.
2. S. H. Pine, *Organic Chemistry*, Tata McGraw Hill, 5th Edition, **2008**.
3. R. Chang, *Chemistry*, 1st Indian Edition, Tata-McGraw Hill, **2007**.
4. *Guidebook to Mechanism in Organic Chemistry* (6th Edition), Peter Sykes, Longman Scientific & Technical, **1985**.
5. *March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure*, Michael B. Smith, Jerry March John Wiley & Sons, sixth edition, **2007**.
6. *Stereochemistry of Organic Compounds*, Ernest L. Eliel, Publisher, Tata McGraw-Hill.

Semester: 3

Subject Code: CHE0302

Credits: 3

0-0-3-2

Title: General Chemistry Practical - II

Understanding error, accuracy and precision by measuring physical parameters

Determination of physical properties of materials

Experiments involving chemical thermodynamics, chemical equilibria, chemical kinetics and electro chemistry

Reference Books

1. Halpern, A. M.; McBane, G. C. *Experimental Physical Chemistry: A Laboratory Prescribed Book*, W. H. Freeman, 3rd edition, **2006**.
2. Hein, M.; Peisen, J. N.; Miner, R. L.; *Foundations of College Chemistry in the Laboratory*, John Wiley & Sons Inc., **2011**.
3. Dave, R. K.; *Experiments in Physical Chemistry*, Campus Books International, **2011**.

Semester: 4

Subject Code: CHE0401

Credits: 2

2-1-0-3

Title: General Chemistry IV

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

Chemical Bonding and Basic Coordination Chemistry: Molecular orbital theory: Homo- and heterodiatomic and polyatomic molecules. Basic coordination chemistry: ligands, coordination complexes - Werner's theory – coordination geometries, isomerism – d-orbital splitting, spectrochemical series, magnetic properties. Metallurgy – Principles only. Basic organometallic chemistry: 18-electron rule, bonding aspects, structures of organometallic compounds.

Hydrogen, Hydrides and Alkali and Alkaline Earth Metals: Hydrogen: Electronic structure, abundance, preparation and properties, isotopes, ortho- and para hydrogens. Hydrides: ionic, covalent, metallic and intermediate hydrides; Hydrogen bonding. Alkali metals: Introduction, halides, oxides and hydroxides, salts of oxo-acids and aqueous solution chemistry. Alkaline Earth metals: Introduction, halides, oxides and hydroxides, salts of oxo-acids, and aqueous solution chemistry

Oxygen Group and Halogen Family – A Basic Treatment: Oxygen group: Introduction – Hydrides; Halides, Oxohalides and complex halides – Oxides, Oxo-acids 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 oxyacids of halogens (structure only) – Basic properties of halogens – Inter-halogen compounds – preparation, properties and uses – Pseudohalogen – Preparation, properties and uses of cyanogens and thiocyanogen comparison with halogens – Anomalous properties of fluorine.

Prescribed Books

1. J. D. Lee, Concise Inorganic Chemistry, 5th Edition, Blackwell Science, **1996**.
2. G. Sharpe, Inorganic Chemistry, 3rd Edition, Pearson, **2010**
3. P. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong, Inorganic Chemistry, 5th Edition, Oxford University Press, **2010**
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**.

Reference Books

1. N. N. Greenwood and A. Earnshaw, Chemistry of the Elements, 2nd Edn., Elsevier, **2005**.
2. C. E. Housecraft and A. G. Sharpe, Inorganic Chemistry, 4th edition, Pearson, **2012**.
3. R. Chang, Chemistry, 1st Indian Edition, Tata-McGraw Hill, **2007**.
4. B. Douglas, D. McDaniel and J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Edition, John Wiley & Sons, **2010**.
5. F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann, Advanced Inorganic Chemistry, 6th Edition, John Wiley & Sons, **2008**.

Semester: 4

Subject Code: CHE0402

Credits: 2

0-0-3-2

Title: General Chemistry Practical - III

1. Melting point determination.
2. Crystallization, Decolorization using Charcoal
3. Qualitative Analysis of simple organic compounds:
The following functional groups are to be analyzed: 1. Aldehydes, 2. Ketones, 3. Phenols, 4. Monocarboxylic acids, 5. Diamides, 6. Amines 7. Carbohydrates and 8. Esters
4. One step preparation of organic compounds by Green route. Crystallization and melting point determination.

Reference Books

1. Vogel's Prescribed book of Practical Organic Chemistry, 5th edition, Pearson Publishers.
2. Experimental Organic Chemistry Vol 1 and 2, P R Singh, D S Gupta, K S Bajpai, Tata McGraw Hill
3. Laboratory Manual in Organic Chemistry, R. K. Bansal, Wiley.
4. Monograph on Green Chemistry Laboratory Experiments, B. C. Ranu (Ed.) Green Chemistry Task Force Committee, DST, New Delhi, **2012**.

Semester: 5

Subject Code: CHE0501

Credits: 4

4-1-0-4

Title: Inorganic Chemistry I

Acids and Bases, Chemistry in 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 leveling effects. Chemistry in aqueous and Non-aqueous Solvents - super acids - molten salts.

Boron Group: Introduction, diborane and hydrogen compounds of the other elements, metal borides, halides and complex halides of B, Al, Ga, In and Tl, oxides, oxo-acids, oxoanions and hydroxides; nitrogen derivatives; Al, Ga, In and Tl salts of oxo-acids and aqueous solution chemistry, organometallic compounds.

Carbon Group: Introduction, Intercalation compounds of graphite, hydrides, carbides and silicides, halides and complex halides; oxides and oxo-acids of carbon; oxides and oxoacids and hydroxides of Si, Ge, Sn and Pb; Silicates; Silicones; Cyanogen, its derivatives and silicon nitride; aqueous solution chemistry and oxo-acid salts of Sn and Pb; Organometallic compounds.

Nitrogen Group: Introduction; hydrides; nitrides, phosphides and arsenides; halides, oxo-halides and complex halides; Oxides, oxo-acids and sulfides of N, P, As, Sb and Bi; Phosphazenes; Aqueous solution chemistry; Organic derivatives.

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

Prescribed Books

1. 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**.
2. P. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong, *Inorganic Chemistry*, 5th Edition, Oxford University Press, **2010**
3. J. D. Lee, *Concise Inorganic Chemistry*, 5th Edition, Blackwell Science, **1996**.
4. G. L. Miessler and D. A. Tarr, *Inorganic Chemistry*, 3rd Edition, Pearson, **2004**.
5. A. G. Sharpe, *Inorganic Chemistry*, 3rd Edition, Pearson, **2010**

Reference Books

1. N. N. Greenwood and A. Earnshaw, *Chemistry of the Elements*, 2nd Edn., Elsevier, **2005**.
2. C. E. Housecraft and A. G. Sharpe, *Inorganic Chemistry*, 4th edition, Pearson, **2012**.
3. A. G. Massey, *Main Group Chemistry*, 2nd edition, John and Wiley & Sons, LTD, **2000**.
4. F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann, *Advanced Inorganic Chemistry*, 6th Edition, John Wiley & Sons, **2008**.
5. B. Douglas, D. McDaniel and J. Alexander, *Concepts and Models of Inorganic Chemistry*, 3rd Edition, John Wiley & Sons, **2010**.

Semester: 5**Subject Code: CHE0502****Credits: 4****4-1-0-4****Title: Structure and reaction mechanisms**

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

Structural effects on stability and reactivity: Thermodynamic stability – general relationships between thermodynamic stability and reaction rates – electronic substituent effects on reaction intermediates – kinetic isotope effects – linear free energy relationship – substituent effects – catalysis – solvent effects.

Nucleophilic substitution: Mechanisms for nucleophilic substitutions – structural and solvation effects on reactivity – Neighboring-Group Participation (NGP) – structure and reactions of carbocation intermediates.

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

Polar addition and elimination reactions: Addition of hydrogen halides to alkenes – acid catalysed hydration and related addition reactions addition to halogens – sulfonylation and selenylation reactions – addition reactions involving epoxides – E1, E2, E1cb and pyrolytic eliminations.

Prescribed Book

1. F.A.Carey and R.J.Sundberg, Advanced Organic Chemistry, Part A: Structure and Mechanisms, 5th edition, 2007.

Reference Books

1. R. T. Morrison, R. N. Boyd and S. K. Bhattacharjee, Organic Chemistry, 7th Edition, Pearson Prentice Hall, **2011**.
2. S. H. Pine, Organic Chemistry, Tata McGraw Hill, 5th Edition, **2008**.
3. Michael B. Smith, Jerry March, March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, John Wiley & Sons, 6th edition, **2007**.
4. I. L. Finar, Organic Chemistry, Vol. I & II, 5th Edition, Longman Ltd., New Delhi, **1975**.
5. D. Nasipuri, Stereochemistry of Organic Compounds: Principles and Applications, 4th edition, New Academic Science Publisher.
6. Peter Sykes, Guidebook to Mechanism in Organic Chemistry (6th Edition), Longman Scientific & Technical, **1985**.
7. Ernest L. Eliel, Stereochemistry of Organic Compounds, Tata McGraw-Hill.

Semester: 5**Subject Code: CHE0503****Credits: 4****4-1-0-4****Title: Kinetics, Surfaces and Interfaces**

Kinetics: Rate, molecularity and order of chemical reactions; unimolecular and bimolecular reactions; Theories of reaction rates: Collision theory, activated complex theory, Lindemann unimolecular theory, studies and kinetics of ultrafast reactions; Theories of unimolecular gaseous reactions; Marcus theory. Complex chemical kinetics: Reversible, concurrent, consecutive reactions. Unimolecular reactions (Lindmann theory), steady-state approximations, theory of absolute reaction rate and its thermodynamic formulation, temperature dependence of frequency factor, numerical problems.

Photochemistry: Basics of Photochemistry and Photophysics, Jablonski diagram. Electronically excited states: electronic, vibrational and spin levels, Born-Oppenheimer approximation, energy quantization, potential energy curves and surfaces, spin: vectorial representation, triplets, singlet and triplet states. laws of photochemistry – Grotthus-Draper law – Stark Einstein's law – Photochemical reactions and kinetics – Energy transfer – photosensitization and quenching – Stern-Volmer's equation.

Catalytic activity at surfaces, Surface area determination (BET equation), transition state theory of surface reactions: rates of chemisorption and desorption, unimolecular and bimolecular surface reactions, comparison of homogeneous and heterogeneous reaction rates, surface heterogeneity, and lateral interaction.

Theory of activity co-efficient of strong electrolytes; Electrified interfaces: theories and models; Basics in Electro-catalysis and Bio-electrochemistry; Kinetics of electrode reactions; Irreversible electrode processes.

Prescribed Books

1. McQuarrie, D. A.; Simon, J. D.; Physical Chemistry: A Molecular Approach, University Science Books, **2011**.
2. Atkins, P. W.; Paula, J.; Physical Chemistry, Oxford Publications, 8th edition, **2009**.
3. Laidler, K. J.; Chemical Kinetics, Pearson Education, 3rd edition, **2011**.
4. Rohatgi-Mukherjee, K. K; Fundamentals of Photochemistry, Wiley Eastern Ltd, **1992**.

Reference Books

1. Hill, T. A.; An Introduction to Statistical Thermodynamics, Dover Publications Inc., **1987**.
2. Levine, I. N.; Physical Chemistry, McGraw-Hill Science/Engineering/Math, 6th edition, **2008**.
3. Turro, T. J.; Ramamurthy, V.; Scaiano, J. C.; Principles of Molecular Photochemistry: An Introduction, University Science Books, 1st edition, **2008**.

Semester: 5

Subject Code: CHE0504

Credits: 4

4-1-0-4

Title: Analytical Chemistry: Instrumental methods of analysis

Error analysis: Errors - Determinant, constant and indeterminate. Accuracy and precision-Distribution of random errors. Average deviation and standard deviation, variance and confidence limits.

Significant figures and computation rules. Least squares method of analysis.

Methods of sampling: sample size, techniques of sampling of gases, fluids, solids, and particulates.

Chromatographic methods: General principles - classification of chromatographic methods - nature of partition forces. Chromatographic behavior of solutes- column efficiency and resolution.

Gas Chromatography: detector, optimization of experimental conditions. Ion-exchange chromatography, thin layer chromatography, coating of materials, preparative TLC.

Solvents used and methods of detection - Column chromatography: Adsorption and partition methods. Nature of column materials-preparation of the column.

Thermo Gravimetric Analysis and Differential Scanning Calorimetry: Effect of heat on materials, Chemical decomposition and T, G curves, Analysis of T, G. curve to show nature of decomposition reactions, the product and qualities of compounds expelled, applications, instrumentation.

DSC- theory, instrumentation and applications - thermometric titrations and applications.

AAS and ICP: Atomic Absorption Spectroscopy- Introduction, Principle, differences between AAS and FES - Advantages of AAS over FES, advantages and disadvantages of AAS. Instrumentation - single and double beam AAS, detection limit and sensitivity, Interferences - applications.

Inductively coupled Plasma Spectroscopy - Nebulization Torch, Plasma, Instrumentation, Interferences, Applications.

Flame photometry: Principle – instrumentation-applications

Electroanalytical techniques: Cyclic voltammetry: Principles, instrumentation, and analytical applications - Differential pulse voltametry and Square wave voltametry.

Polarography: Introduction, Instrumentation, Ilkovic equation and its verification. Determination of half-wave potential, qualitative and quantitative applications.

Amperometry: Basic principles, instrumentation, nature of titration curves, and analytical applications.

Prescribed Books

1. H. H. Willard, L. L. Merritt, and J. A. Dean, Instrumental Methods of analysis, CBS Publishers & Distributors, Shahdara, Delhi, 6th edition, **1986**.
2. D. Skoog and D. West, Principles of Instrumental Analysis, Cengage Learning; 6th edition, **2006**.

Reference Books

1. Gary D. Christian, Analytical Chemistry, John Wiley & Sons, 6th edition, **2007**.
2. J. M. Bobbitt, Roy Gritter, Introduction to chromatography, Holden Day; 2nd edition, **1985**.
3. Gurdeep R. Chatwal, Sham K. Anand, Instrumental Methods of Analysis, Himalaya Pub., **1979**.
4. G. Svehla: *Vogel's qualitative inorganic analysis*, 7th Edition, Prentice Hall, **1996**.
5. Howard A. Strobel, William R. Heineman, Chemical Instrumentation: A Systematic approach, Wiley-Interscience; 3 edition, **1989**.
6. W.E. Morf, The principles of ion-selective electrodes and membrane transport, Elsevier Science Ltd, **1981**.
7. Atkins, P. W.; Paula, J.; Physical Chemistry, Oxford Publications, 8th edition, **2009**.
8. I.M. Kolthoff, Treatise on Analytical Chemistry, Wiley Interscience, Vol I to VII.

Semester: 5

Subject Code: CHE0505

Credits: 3

0-1-5-3

Title: Inorganic and Analytical Chemistry Techniques

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

Volumetric and Gravimetric experiments

A mixture of solution(s) should be given for estimation

- | | |
|----------------------|----------------------|
| 1. Cu (V) and Ni (G) | 4. Fe (V) and Ni (G) |
| 2. Cu (V) and Zn (G) | 5. Zn (V) and Cu (G) |
| 3. Fe (V) and Zn (G) | |

Reference Books

1. G. Svehla: *Vogel's qualitative inorganic analysis*, 7th Edition, Prentice Hall, **1996**
2. J. Mendham, R. C. Denney, J. D. Barnes, M. J. K. Thomas: *Vogel's Prescribed book of qualitative chemical analysis*, 6th Edition, Prentice Hall, **2000**.
3. J. D. Woollins, *Inorganic experiments*, 3rd Edition, Wiley-VCH Verlag GmbH @Co. KGaA, **2012**.
4. M. Hein, J. N. Peisen and R. L. Miner, *Foundations of College Chemistry in the Laboratory*, John Wiley and Sons, **2011**

5. Jeffery G H, Bassett J, Mendham J, Denney R C, *Vogel's Prescribed Book of Inorganic Quantitative Analysis*, Longman, **1984**.
6. A. J. Elias, *A Collection of Interesting General Chemistry Experiments*, Universities Press, Sangam Books Ltd, **2002**.

Semester: 5

Subject Code: CHE0506

Credits: 3

0-1-5-3

Title: Organic Chemistry Lab I

1. Thin Layer Chromatography: Determination of R_f- values and identification of organic compounds.
2. One step organic preparations: TLC, crystallization, melting point determination.
3. Steam Distillation
4. Column chromatography
5. Qualitative Analysis : Separation and analysis of organic mixture containing two components and preparation of suitable derivatives.

Reference Books

1. P R Singh, D S gupta, K S Bajpai, *Experimental Organic Chemistry Vol 1 and 2*, Tata McGraw Hill
2. R. K. Bansal, *Laboratory Manual in Organic Chemistry*, Wiley, **2006**.
3. A.I. Vogel , A.R. Tatchell, B.S. Furnis , A.J. Hannaford , P.W.G. Smith, *Vogel's Prescribedbook of Practical Organic Chemistry*, 5th Edition, Pearson education Ltd, **1996**.

Semester: 6

Subject Code: CHE0601

Credits: 4

4-1-0-4

Title: Inorganic Chemistry II

Solid State Chemistry I: Ionic solids, close packing, radius ratio rules, Structures of ionic crystals – AX and AX₂ type crystal structures – layer structures - lattice energy - Born-Lande, Born-Mayer and Kapustinskii equations – Derivations and applications – Decomposition of ionic solids – solubility of ionic solids

Solid State Chemistry II: Defects and Non-stoichiometric - Intrinsic and extrinsic defects - point, line and plane defects; vacancies, Stoichiometric defects - Schottky and Frenkel defects - Non-stoichiometry – Metal excess and Metal-deficiency - thermodynamic and structural aspects. n- and p-type semiconductors – photovoltaic cell - Transistors – superconductivity.

Nuclear Chemistry: Introduction – composition of nucleus and nuclear forces.

Nuclear stability – o/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.

Radioactivity and Nuclear Transformations: 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. Applications of radio isotopes – Carbon dating – Radioactive waste disposal. Radiolysis of water and hydrated electron.

Oxidation and Reduction - Redox Potentials: Nernst Equation, Electrochemical series, Use of redox potential data – analysis of redox cycle, - Standard reduction potentials, E° , relationship between E° , ΔG° and K , Formal Potential and its application: Effect of pH, complexation, solubility; Disproportionation and comproportionation reaction, Redox stability in water: Frost-Ebsworth, Latimer and Pourbaix diagrams, applications of redox reactions to extraction of elements from their ores: Ellingham diagrams.

Prescribed Books

1. J. E. Huheey, E. A. Keiter, R. L. Keiter and O. K. Medhi, *Inorganic Chemistry - Principles of Structure and Reactivity*, 4th Edition, Pearson Education, **2006**.
2. P. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong, *Inorganic Chemistry*, 5th Edition, Oxford University Press, **2010**
3. J. D. Lee, *Concise Inorganic Chemistry*, Fifth Edition, Wiley-India, **2010**.
4. S. Glasstone, 'Source Book on Atomic Energy', 3rd edn., Affiliated East West Press, **1979**.

Reference Books

1. G. L. Miessler and D. A. Tarr, *Inorganic Chemistry*, 3rd Edition, Pearson, **2004**.
2. E. S. Gilreath, 'Fundamental concepts of Inorganic Chemistry', International students edn., McGraw-Hill Kogakusha, Ltd., **1958**.
3. G. Chatwal and M. S. Yadu, 'Co-ordination Chemistry', First edn., Himalaya Publishing House, **1992**.
4. B. Douglas, D. McDaniel and J. Alexander, *Concepts and Models of Inorganic Chemistry*, 3rd Edition, John Wiley & Sons, **2010**.
5. F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann, *Advanced Inorganic Chemistry*, 6th Edition, John Wiley & Sons, **2008**.
6. M. C. Day Jr and J. Selbin, *Theoretical Inorganic Chemistry*, Literary Licensing, LLC, **2012**
7. H. E. Boyer, and T. L. Gall, *Metals Handbook*, Desk Edition, **1984**
8. W. D. Loveland, D. J. Morrissey, G. T. Seaborg, *Modern Nuclear Chemistry*, Wiley-VCH Verlag GmbH Co. KGaA, **2006**.

Semester: 6

Subject Code: CHE0602

Credits: 4

4-1-0-4

Title: Reaction mechanism and organic photochemistry

Addition, condensation and substitution reactions of carbonyl compounds: Reactivity of carbonyl compounds towards addition – hydration and addition of alcohols to aldehydes and ketones – condensation reactions of aldehydes and ketones with nitrogen nucleophiles – substitution reactions of carboxylic acid derivatives – intramolecular catalysis of carbonyl substitution reactions – addition

of organometallic reagents to carbonyl groups – addition to enolates and enols to carbonyl compounds: Aldol addition and condensation reactions.

Aromaticity: Criteria of aromaticity – non-benzenoid aromatic compounds – anti-aromaticity, homo aromaticity – fused-ring systems –hetero aromatic systems.

Aromatic substitution reactions: Electrophilic aromatic substitution reactions – structure-reactivity relationships for substituted benzenes – reactivity of polycyclic and heteroaromatic compounds – specific electrophilic substitution reactions – nucleophilic aromatic substitution reactions – VNS - transition metal- catalyzed aromatic substitution reactions – aromatic substitution reactions involving radical intermediates.

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

Prescribed Books

1. F.A.Carey and R.J.Sundberg, Advanced Organic Chemistry, Part A: Structure and Mechanisms, 5th edition, **2007**.
2. March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, Michael B. Smith, Jerry March John Wiley & Sons, 6th edition, **2007**.
3. N. J. Turro , J.C. Scaiano and V. Ramamurthy, Modern Molecular Photochemistry of Organic Molecules, University Science Books, **2010**.

Reference Books

1. R. T. Morrison, R. N. Boyd and S. K. Bhattacharjee, Organic Chemistry, 7th Edition, Pearson Prentice Hall, **2011**.
2. S. H. Pine, Organic Chemistry, Tata McGraw Hill, 5th Edition, **2008**.
3. Guidebook to Mechanism in Organic Chemistry (6th Edition), Peter Sykes, Longman Scientific & Technical, **1985**.
4. The Art of Writing Reasonable Organic Reaction Mechanisms, Robert B. Grossman, second edition, Springer, **2010**.
5. P.S. Kalsi, Organic Reactions and Their Mechanisms, 1st Edition, New Age International Pub., New Delhi, **1996**.
6. I. L. Finar, Organic Chemistry, Vol. I & II, 5th Edition, Longman Ltd., New Delhi, **1975**.

Semester: 6

Subject Code: CHE0603

Credits: 4

4-1-0-4

Title: Introductory Quantum Chemistry

Discovery of electron, Black body radiation, Photo-electric effect, Planck's Quantum hypothesis, Hydrogen atomic spectra, Quantization of angular momentum, Wave-particle duality - Bohr theory, de Broglie postulation of matter, Heisenberg uncertainty Principle.

Principles of classical mechanics and the experimental evidence of its inadequacies, Wave-particle duality and uncertainty principle.

Wave equation, wave functions, properties of wave functions, Normalization of wave functions, orthogonality of wave functions, one dimensional wave equation, separation of variables for solving wave equation, general solutions to wave equations, two dimensional wave equations.

Wave function of a particle - Schrödinger equation, Eigen value problem, linear operators classical mechanical quantities in quantum mechanics, probabilistic interpretation, energy of a particle in a box, wave function normalization, variance, continuous probability distribution, average momentum of a particle in a box, particle in a one dimensional box.

Representation of a state of a system by wave function, quantum mechanical operators-classical mechanical variables, time dependence of wave function, time dependent Schrödinger equation, Hermitian operators, Eigen functions of Hermitian operators, orthonormal sets

Hooke's law, Harmonic oscillator, energy of harmonic oscillator, equation for a harmonic oscillator-diatomic molecule- reduced mass, energy levels of a quantum mechanical harmonic oscillator, IR spectra of diatomic molecule, hermite polynomials, kinetic and potential energy of a harmonic oscillator, Hermite differential equations, Relations among Hermite polynomials.

Extension of one dimensional box - problem of a particle in a three dimensional box, separation of Hamiltonian- Eigen functions and Eigen values, Laplacian coordinators, rigid rotor, energy levels of a rigid rotor, spherical harmonics, Schrödinger equation for the hydrogen atom – solutions, s orbitals, p orbitals, energy levels of a hydrogen atom in magnetic field, Schrödinger equation for Helium atom.

Prescribed Books

1. McQuarrie, D.; Quantum chemistry, University Science Publishers, **2007**.
2. McQuarrie, D. A.; Simon, J. D.; Physical Chemistry: A Molecular Approach, University Science Books, **2011**.
3. Prasad, R. K.; Quantum Chemistry, New Age International Publishers, 4th edition, **2010**.

Reference Books

1. Raff, L. M.; Principles of Physical Chemistry, Prentice Hall, **2001**.
2. Atkins, P. W.; Paula, J.; Physical Chemistry, Oxford Publications, 8th edition, **2009**.
3. Levine, I. N.; Physical Chemistry, McGraw-Hill Science/Engineering/Math, 6th edition, **2008**.
4. Kreyszig, Advanced Engineering Mathematics, 9th Edition, **2012**.

Semester: 6

Subject Code: CHE0604

Credits: 4

4-1-0-4

Title: Solutions and Soft Matter

Solutions: Introduction to solution: liquids in liquids; Ideal solutions and Raoult's law; Concepts of activity and fugacity and activity coefficients; Non ideal solutions; Gibbs-Duhem-Margules equation, Henry's law; Azeotropic mixtures, Introduction to completely miscible binary solutions and partially miscible liquids colligative properties: Freezing point depression, elevation of boiling point, osmotic pressure. van't Hoff equation and van't Hoff factor. Measurement of osmotic pressure and applications

Solid solutions, solubility limit, phase rule, binary phase diagrams, intermediate phases, intermetallic compounds, Alloys

Colloids and interface: classification, preparation and purification of colloids; properties of colloidal systems; electrical properties – charge, electrical double layer; DLVO theory, electrokinetic properties: electrophoresis, electroosmosis; Optical and Physical properties, determination of size of colloidal particles involving microscopy, scattering (LS, DLS, x-ray, neutron), sedimentation, centrifugation, chromatography, acoustics, adsorption.

Interphase region, curved surfaces. Thermodynamics of surfaces : Gibbs adsorption isotherm, heat and entropy of adsorption. Surface film on liquids; Electro-kinetic phenomena.

Gels - definition - Thermoreversible and Irreversible Physical Gels - inorganic gels - Small molecule organo gelators - associating Polyelectrolyte gels - polyelectrolyte gels - electrical behaviors and mechanical responses of polyelectrolyte gels.

Prescribed Books

1. Silbey, R. J.; Albert, R. A.; Bawendi, M. G.; Physical Chemistry, Wiley, 4th edition, **2004**.
2. R. Chang, Chemistry, 1st Indian Edition, Tata-McGraw Hill, **2007**.
3. Atkins, P. W.; Paula, J.; Physical Chemistry, Oxford Publications, 8th edition, **2009**.

Reference Books

1. Castellan, G. W.; Physical Chemistry, Narosa Publishing House, 3rd edition, **2004**.
2. Raff, L. M.; Principles of Physical Chemistry, Prentice Hall, **2001**.
3. Laidler, K. L.; Chemical Kinetics, Pearson Education Inc, 3rd edition, **2011**.
4. Levine, I. N.; Physical Chemistry, McGraw-Hill Science/Engineering/Math, 6th edition, **2008**.
5. Shillady, D.; Essentials of Physical Chemistry, CRC Press, **2012**.

Semester: 6

Subject Code: CHE0605

Credits: 3

0-1-5-3

Title: Physical Chemistry Practical I

Advanced experiments involving chemical thermodynamics, chemical equilibria, chemical kinetics and electro chemistry

Reference Books

1. Halpern, A. M.; McBane, G. C. Experimental Physical Chemistry: A Laboratory Prescribed Book, W. H. Freeman, 3rd edition, **2006**.
2. Viswanathan, B.; Raghavan, P. S.; Practical Physical Chemistry, Viva Books, **2010**.
3. Hein, M.; Peisen, J. N.; Miner, R. L.; Foundations of College Chemistry in the Laboratory, John Wiley & Sons Inc., **2011**.
4. Dave, R. K.; Experiments in Physical Chemistry, Campus Books International, **2011**.

Semester: 6

Subject Code: CHE0606

Credits: 3

0-1-5-3

Title: Organic Chemistry – Lab

Quantitative analysis

1. Estimation of Phenol and aniline - volumetric method.
2. Estimation of glucose by Betrand's method.
3. Estimation of methyl ketone – iodimetric method
4. Determination of the percentage or number of hydroxyl groups in organic compounds by acetylation method.
5. Determination of iodine and saponification value of an oil sample.
6. Estimation of nitrogen by Kjeldahl analysis.
7. Estimation of carbonyl group using 2, 4 – DNP.
8. Estimation of halogens
9. Estimation of phenol using spectrophotometric method.

Reference Books:

1. A.I .Vogel, Elementary Practical Organic Chemistry: Small Scale Preparations, Qualitative Organic Analysis, Quantitative Organic Analysis.
2. J. Leonard , B. Lygo G. Procter, Advanced Practical Organic Chemistry, 3rd edition, CRC press, **2013**.
3. Experimental Organic Chemistry Vol 1 and 2, P R Singh, D S Gupta, K S Bajpai, Tata McGraw Hill
4. Laboratory Manual in Organic Chemistry, R. K. Bansal, Wiley. **2006**.

Semester: 7

Subject Code: CHE0701

Credits: 4

4-1-0-4

Title: Inorganic Chemistry III

The Chemistry of the Main Group Elements: Periodicity- First- and Second-Row Anomalies, Use of p-orbitals in pi bonding, pπ- pπ bonding in heavier main group elements - Use (or not) of d orbitals by nonmetals, reactivity of d-orbital participation, periodic anomalies of the nonmetals and post transition metals.

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.

Coordination Chemistry: Studies of coordination compounds in solution – detection of complex formation in solution – Stability constants – stepwise and over-all formation constants – simple methods (Potentiometric, pH metric and photometric methods) of determining the formation constants - Factors affecting stability – statistical and chelate effects – Forced configurations.

Theories of Metal-Ligand Bond: VB theory and its limitations – Crystal field theory - splitting of d-orbitals under various geometries – Factors affecting splitting – CFSE and evidences for CFSE (Structural and thermodynamic effects) – Spectrochemical series – Jahn-Teller distortion – Spectral and magnetic properties of complexes – Site preferences - Limitations of CFT – Ligand field theory – MO theory – sigma – and pi-bonding in complexes – Nephelauxetic effect – The angular overlap model.

Coordination Chemistry – 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 – electron exchange reactions – complementary and non-complementary types – inner sphere and outer sphere processes – Application of Electron transfer reactions in inorganic - isomerisation and racemisation reactions of complexes – Molecular rearrangement – Reactions of four and six-coordinate complexes – Interconversion between stereoisomers. Reactions of coordinated ligands – Template effect and its application for the synthesis of Macrocyclic ligands – Unique properties – Cr-Cr quintable bond.

Inorganic Photochemistry: Electronic transitions in metal complexes, metal-centered and charge-transfer transitions – Various photophysical and photochemical processes of coordination compounds

Unimolecular charge-transfer photochemistry of cobalt(III) complexes. Mechanism of CTTM photoreduction. Ligand-field photochemistry of chromium(III) complexes, Adamson's rules, photoactive excited states, V-C model – photophysics and photochemistry of ruthenium-polypyridine complexes, emission and redox properties – photochemistry of organometallic compounds, metal carbonyl compounds, compounds with metal-metal bonding Reinecke's salt - chemical actinometer.

Prescribed Books

1. 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**.
2. P. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong, *Inorganic Chemistry*, 5th Edition, Oxford University Press, **2010**.
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*, 4th ed., A Wiley - Interscience Publication, John -Wiley & Sons, USA.
5. W. Adamson and P. D. Fleischauer, *Concepts of Inorganic Photochemistry*, Wiley, New York, **1975**.

Reference Books

1. M. C. Day and J. Selbin, *Theoretical Inorganic Chemistry*, Affiliated East West Press Pvt. Ltd. 2nd ed., **1985**.
2. S. F. A. Kettle, *Physical Inorganic Chemistry – A Coordination Chemistry Approach*, Spectrum Academic Publishers, Oxford University Press, **1996**.
3. J. Ferraudi, *Elements of Inorganic Photochemistry*, Wiley, New York, **1988**.
4. F. Basolo and R. G. Pearson, *Mechanism of Inorganic Reactions*, John Wiley, New York.
5. G. L. Miessler and D. A. Tarr, *Inorganic Chemistry*, 3rd Edition, Pearson, **2004**.
6. C. E. Housecraft and Alan G. Sharpe, *Inorganic Chemistry*, 4th edition, Pearson, **2012**.

7. K. F. Purcell and J. C. Kotz, *Inorganic Chemistry*, Saunders Golden Sunburst Series, W. B. Saunders Company, Philadelphia, **1977**.
8. M. C. Day Jr and J. Selbin, *Theoretical Inorganic Chemistry*, Literary Licensing, LLC, **2012**
9. G. Wilkinson, R. D. Gillars and J. A. McCleverty, *Comprehensive Co-ordination Chemistry*, Pergamon Press, **1987**.
10. G. Wulfborg, *Inorganic Chemistry*, University Science Books, **2000**.

Semester: 7**Subject Code: CHE0702****Credits: 4****4-1-0-4****Title: Reaction mechanism and reactivity**

Heterocycles II: Heterocyclics with more than one hetero atom – Introduction to fused five and six membered heterocyclics – preparation and reaction of indole, quinoline, isoquinoline and carbozole.

Reactions of carbon nucleophiles with carbonyl compounds: Aldol addition and condensation reactions – addition reactions of imines and iminium ions – acylation of carbon nucleophiles – olefination reactions of stabilized carbon nucleophiles – reactions proceeding by addition-cyclisation – conjugate addition by carbon nucleophiles.

Functional group interconversion by substitution (including protection and deprotection strategies): Conversion of alcohols to alkylating agents – introduction of functional groups by nucleophilic substitution at saturated carbon – cleavage of carbon-oxygen bonds in ethers and esters – inter conversion of carboxylic acid derivatives – installation and removal of protective groups.

Electrophilic additions to carbon-carbon multiple bonds: Electrophilic cyclization – electrophilic substitution to carbonyl groups – additions to allenes and alkynes – addition at double bonds via organoborane intermediates – hydroalumination, carboalumination, hydrozirconation and related reactions.

Reduction of carbon-carbon multiple bonds, carbonyl groups and other functional groups: Addition of hydrogen at carbon-carbon multiple bonds – catalytic hydrogenation of carbonyl and other functional groups – group-III hydride-donor reagents – group-IV hydride donors – reduction reactions involving hydrogen atom donors – dissolving-metal reductions – reductive deoxygenation of carbonyl groups – reductive elimination and fragmentation.

Prescribed texts

1. F.A.Carey and R.J.Sundberg, *Advanced Organic Chemistry, Part B: Reactions and synthesis*, Springer, 5th edition, **2007**.

Reference books

1. R. T. Morrison, R. N. Boyd and S. K. Bhattacharjee, *Organic Chemistry*, 7th Edition, Pearson Prentice Hall, **2011**.
2. S. H. Pine, *Organic Chemistry*, Tata McGraw Hill, 5th Edition, **2008**.
3. W. Carruthers and I. Coldham, *Modern methods of Organic Synthesis*, Cambridge University Press, First South Asian Edition, **2005**.
4. J. March and M. B. Smith, *March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure*, 6th Edition, Wiley, **2007**.
5. *Organic Synthesis*, Oxford Chemistry Primers, 31, C. L. Willis, M. Wills, Oxford Science Publications, **1996**.

6. Introduction to Strategies for Organic Synthesis, Laurie S. Starkey, Wiley, **2012**.
7. March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, Michael B. Smith, Jerry March John Wiley & Sons, 6th edition, **2007**.

Semester: 7**Subject Code: CHE0703****Credits: 4****4-1-0-4****Title: Symmetry and Group Theory of Molecules**

A systematic procedure for symmetry classification of molecules. Symmetry elements, symmetry operations, Representation of Groups, Matrix representation of symmetry operations, reducible and irreducible representations, orthogonality theorem.

Construction of character tables for point groups C_{2v}, C_{3v} and D_{2h}, structure of character tables, determination of symmetry species for translations and rotations.

Concepts of Groups, Sub-groups, Classes of Symmetry operations, Group Multiplication Tables. Abelian and non-Abelian point groups. Symmetry criterion of optical activity, symmetry restrictions on dipole moment

Group theory and Quantum Mechanics, Perturbation theory, Variational methods, Hartree-Fock equations, Self-consistent field methods for solving Hartree-Fock equations, Term symbols and electronic configuration, Russel-Saunders coupling, 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, sp² and sp³ hybrid orbitals, molecular term symbols, Hückel molecular orbitals, bonding in polyatomic molecules.

Prescribed Books

1. Cotton, F. A.; Chemical Applications of Group Theory, John Wiley & Sons Inc., 3rd edition, **2009**.
2. McQuarie, D.; Quantum chemistry, University Science Publishers, **2007**.
3. McQuarie, D. A.; Simon, J. D.; Physical Chemistry: A Molecular Approach, University Science Books, **2011**.

Reference Books

1. Jaffe, H. H.; Orchin, M.; Symmetry in Chemistry, John Wiley & Sons Inc., 2002.
2. Atkins, P. W.; Paula, J.; Physical Chemistry, Oxford Publications, 8th edition, **2009**.
3. Levine, I. N.; Physical Chemistry, McGraw-Hill Science/Engineering/Math, 6th edition, **2008**.
4. Raff, L. M.; Principles of Physical Chemistry, Prentice Hall, **2001**.
5. I. N. Levine, Molecular Spectroscopy, John Wiley, **1975**.
6. Harris, D. C.; Bertolucci, M. D.; Symmetry and Spectroscopy: An Introduction to Vibrational and Electronic Spectroscopy, Dover Publications, **1989**.

Semester: 7

Subject Code: CHE0704

Credits: 4

4-1-0-4

Title: Physical methods in organic chemistry

UV- Visible Spectroscopy: Basic principles of electronic transition – Absorption spectra of conjugated dienes and, – unsaturated aromatic carbonyl compounds – Woodward – Fieser rules, effect of solvent polarity on λ_{max} – Applications.

CD and ORD: Cotton effect, ORD, CD - haloketone rule – Application of ORD – CD to stereochemical assignments.

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.

^1H -NMR Spectroscopy: Basic principles- Introduction to NMR techniques – CW and FT NMR techniques. ^1H NMR Spectral parameters – intensity, chemical shift, multiplicity, coupling constant, factors affecting. Analysis of first order and second - order spectra – shift reagents - structure determination of organic compounds by ^1H NMR spectra.

Multinuclear NMR (with specific emphasis on ^{13}C NMR): ^{13}C NMR: Proton coupled; off-resonance decoupled; proton noise decoupled ^{13}C NMR spectra. Assignment of chemical shifts, additivity 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 $^1\text{H} - ^1\text{H}$ COSY, $^1\text{H} - ^{13}\text{C}$ COSY – HMBC, NOESY and INADEQUATE spectra.

Mass Spectrometry: Basic principle – instrumentation- production of ions, EI, CI, FAB – molecular ion peak, Base peak, meta stable peak-nitrogen rule – even electron rule- McLafferty rearrangement – isotopic peaks – Retro Diels Alder reaction – fragmentation pattern of simple organic compounds.

Problems involving interpretation of spectral details of organic compounds.

Prescribed books

1. R. M. Silverstein and F. X. Webster, Spectrometric identification of organic compounds., John Wiley and Sons.Inc., 6th edition, **1997**.
2. W. Kemp, Organic Spectroscopy, 3rd Edition, MacMillon, **1994**.
3. Organic Spectroscopy: Principles & Applications, Jag Mohan, Narosa Publishers, **2012**.

Reference Books

1. Pavia, Lampman and Kriz, Introduction to Spectroscopy, Brooks/Cole Pubs Co, 3rd Edition,
2. D. H Williams and Ian Fleming, Spectroscopic methods in organic chemistry, Tata McGraw Hill, **1998**.
3. NMR in chemistry: A multinuclear introduction. William Kemp, MacMillan, **1988**.
4. Organic Spectroscopy by L. D. S. Yadav, Kulwer academic publishers, **2004**.
5. Electron Spin Resonance Spectroscopy for Organic Radicals by Fabian Gerson and Walter Huber, Wiley-VCH, first edition, **2001**.

Semester: 7

Subject Code: CHE0705

Credits: 3

0-1-5-3

Title: Advanced Organic Synthesis Laboratory

Multistep Organic Synthesis- Conventional synthesis - microwave assisted synthesis- enzymatic reactions - Photochemical reactions. Purification of the compounds using column chromatography and characterization of the compounds using MS, IR, ¹H, ¹³C, and 2D- NMR techniques.

Extraction of Organic compounds from natural sources: Caffeine from Tea leaves- Casein from Milk Nicotine as dipicrate from tobacco- β-carotenes from carrots - Piperine from pepper.

Reference Books:

1. A.I .Vogel, Elementary Practical Organic Chemistry: Small Scale Preparations, Qualitative Organic Analysis and Quantitative Organic Analysis.
2. Advanced Practical Organic Chemistry, J. Leonard , B. Lygo G. Procter, third edition, CRC press, **2013**.
3. P R Singh, D S Gupta, K S Bajpai, Experimental Organic Chemistry Vol 1 and 2, Tata McGraw Hill
4. Laboratory Manual in Organic Chemistry, R. K. Bansal, Wiley. **2006**.
5. R. M. Silverstein and F. X. Webster, Spectrometric identification of organic compounds, John Wiley and Sons.Inc., 6th edition, **1997**.

Semester: 7

Subject Code: CHE0706

Credits: 3

0-1-5-3

Physical Chemistry Laboratory II

Advanced experiments on thermodynamics, kinetics, catalysis, electrochemistry, spectroscopy, photochemistry and macromolecules.

Reference Books

1. In-house laboratory manual
2. Halpern, A. M.; McBane, G. C. Experimental Physical Chemistry: A Laboratory Prescribed Book, 3rd ed.; W. H. Freeman, **2006**.

Semester: 8

Subject Code: CHE0801

Credits: 4

4-1-0-4

Title: Bioinorganic Chemistry and Inner-transition elements

General Principles of Bioinorganic Chemistry: Occurrence and availability of Inorganic elements in biological systems.

Biominalisation:Control and assembly of advanced materials in Biology - Nucleation and crystal growth – various biominerals – calcium phosphate – calcium carbonate – Amorphous silica, Iron biominerals – strontium and barium sulphate.

Function and Transport of Alkali and Alkaline earth metals: Function and Transport of Alkali and Alkaline Earth Metal Ions: Characterization of K^+ , Na^+ , Ca^{2+} and Mg^{2+} - complexes of alkali and alkaline earth metal ions with macrocycles - Ion channels – ion pumps. Catalysis and regulation of bioenergetics processes by the Alkaline Earth Metal ions Mg^{2+} and Ca^{2+} - Pace makers.

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 .

Metalloproteins: Cobalamines: Reactions of the alkyl cobalamins – One-electron Reduction an Oxidation – Co-C Bond Cleavage – coenzyme B_{12} – Alkylation reactions of methylcobalamin.

Heme and Non-heme Proteins: Hemoglobin and Myoglobin – Oxygen transport and storage – Electron transfer and Oxygen activation. Cytochromes, Ferredoxins and Rubredoxins – Model systems, mononuclear non-heme iron enzymes.

Copper Containing Proteins: Classification and examples - Electron transfer – Oxygen transport - Oxygenation – oxidases and reductases – Cytochrome c oxidase – Superoxide dismutase (Cu, Zn).

Nickel containing Enzyme: Urease.

Medicinal Bioinorganic Chemistry: Bioinorganic Chemistry of quintessentially toxic metals. Lead, Cadmium, Mercury, Aluminium, Chromium, Iron, Copper, Plutonium. Detoxification by metal chelation. Drugs that act by binding at the metal sites of Metalloenzymes.

Chemotherapy: Chemotherapy with compounds of certain non-essential elements. Platinum complexes in Cancer therapy – Cisplatin and its mode of action – Cytotoxic compounds of other metals – Gold containing drugs as anti-rheumatic agents and their mode of action - Lithium in Psycho-pharmacological drugs. Radiopharmaceuticals – Technetium.

Inner Transition elements: Special features of f-block elements, introduction, occurrence, separation, oxidation states, lanthanide contraction, coordination number, structures, and simple reactions. Spectral, Magnetic properties and Analytical applications.

Prescribed Books

1. S. J. Lippard and J. M. Berg, *Principles of Bioinorganic Chemistry*, Panima Publishing Company, New Delhi, **1997**.
2. W. Kaim and B. Schwederski, *Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life*, John Wiley & Sons, New York, USA.
3. I. Bertini, H. B. Gray, S. J. Lippard and J. S. Valentine, *Bioinorganic Chemistry*, 1st South Asia Edition, Viva books Pvt. Ltd., **2007**.
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. P. Behrens, E. Bauerlein, *Hand Book of Biomineralization*, 1st Edition, Vol. 1& 2, Wiley-VCH, **2007**.

Reference Books

1. K. F. Purcell and J. C. Kotz, *Inorganic Chemistry*, Saunders Golden Sunburst Series, W. B. Saunders Company, Philadelphia, **1977**.

- Cotton and Wilkinson, *Advanced Inorganic Chemistry*, Wiley Interscience Publication, John Wiley & Sons, New York, USA, 5th ed.,.
- Chem. Education, 62, No. 11, 1985, *Bioinorganic Chemistry*, State of the Art.
- G. L. Eichorn, *Inorganic Biochemistry, Volumes 1 & 2*, 2nd ed., Elsevier Scientific Publishing Company, New York, **1973**.
- F. A. Cotton and G. Wilkinson, *Inorganic Chemistry*, John Wiley & Sons, New York.
- P. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong, *Inorganic Chemistry*, 5th Edition, Oxford University Press, **2010**
- A. Lehninger, D. L. Nelson, Cox, M. M. *Principles of Biochemistry*, 5th Edition, W.H Freeman, **2008**
- E. Alessio, *Bioinorganic Medicinal Chemistry, 1st Edition*, Wiley-VCH Verlag GmbH Co. KGaA, **2012**.

Semester: 8

Subject Code: CHE0802

Credits: 4

4-1-0-4

Title: Reagents and Organic reaction mechanisms

Concerted cycloaddition, unimolecular rearrangements and thermal eliminations: Diels-Alder reactions – 1,3-dipolar cycloaddition reactions – [2+2] cycloadditions and related reactions leading to cyclobutanes – [3,3]-sigmatropic rearrangements – [2,3]-sigmatropic rearrangements – unimolecular thermal elimination reactions. Analysis of pericyclic reactions – orbital correlation diagram – FMO.

Organometallic compounds of Group-I and II metals: Preparation and properties of organomagnesium and organolithium reagents – reactions of organomagnesium and organolithium compounds – organometallic compounds of group IIB and IIIB metals – organolanthanide reagents.

Reactions involving transition metals: Organo-copper intermediates – reactions involving organo-palladium intermediates – reactions involving other transition metals – olefin metathesis reaction – organometallic compounds with pi-bonding.

Oxidation reactions: Oxidation of alcohols to aldehydes, ketones or carboxylic acids – addition to oxygen at carbon-carbon double bonds – allylic oxidation – oxidative cleavage of carbon-carbon double bonds – oxidation of ketones and aldehydes – selective oxidative cleavages at functional groups.

Prescribed books

- F.A.Carey and R.J.Sundberg, *Advanced Organic Chemistry, Part B: Reactions and synthesis*, 5th edition, **2007**.
- Fleming, *Pericyclic Reactions*, Oxford University Press, Oxford, **1999**.
- S.M. Mukherjee and S.P. Singh, *Pericyclic Reactions*, MacMillan India, New Delhi.
- S. Sankararaman, *Pericyclic Reactions - Applications and Theory*, Wiley – VCH, **2005**.

Reference books

- R. T. Morrison, R. N. Boyd and S. K. Bhattacharjee, *Organic Chemistry*, 7th Edition, Pearson Prentice Hall, **2011**.
- S. H. Pine, *Organic Chemistry*, Tata McGraw Hill, 5th Edition, **2008**.
- March's *Advanced Organic Chemistry: Reactions, Mechanisms, and Structure*, Michael B. Smith, Jerry March John Wiley & Sons, 6th edition, **2007**.

4. I. L. Finar, Organic Chemistry, Vol. I & II, 5th Edition, Longman Ltd., New Delhi, **1975**.
5. Guidebook to Mechanism in Organic Chemistry (6th Edition), Peter Sykes, Longman Scientific & Technical, **1985**.
6. S.M. Mukherjee and S.P. Singh, Reaction Mechanism in Organic Chemistry, 1st Edition, Macmillan India Ltd., New Delhi, **1990**.
7. T.H. Lowry and K.S. Richardson, Mechanism and Theory in Organic Chemistry, 3rd Edition, Addison – Wesley Longman Inc., **1998**.

Semester: 8

Subject Code: CHE0803

Credits: 4

4-1-0-4

Title: Introduction to Molecular Spectroscopy

Introduction to spectroscopy and Microwave spectroscopy

Characterization of electromagnetic radiation, energy quantization, spectra and basics of a spectrophotometer, width and intensity of spectral transitions, atomic and molecular spectra, emission and absorption spectra; resolving power, Fourier transformed spectroscopy, Lasers
Microwave spectroscopy, rotation spectra of di – and poly- atomic molecules; Stark effect; Applications of microwave spectra.

IR Spectroscopy

Vibrational spectra of diatomic molecules; simple harmonic oscillator; Hookes law of potential energy; fundamental Vibrational frequency; anharmonic constants; Rotation-vibration spectra of diatomic molecules; Vibrational spectra of diatomic and ploy atomic molecules; breakdown of Born-Oppenheimer approximation, basic instrumentation, vibrational frequencies applicationsof IR spectroscopy

Raman Spectroscopy

Introduction: Quantum theory of Raman scattering, Raman shifts, Rotational Raman spectra, Vibrational Raman Spectra, polarization of light, of Raman spectroscopy, introduction to Resonance Raman spectroscopy; Surface enhanced Raman spectroscopy; Application of Raman spectroscopy

Electronic Spectroscopy

Electronic energy levels-structure of atom; Franck-condon principle; Born – Oppenheimer approximation, electronic spectra of diatomic molecules, electronic spectra of polyatomic molecules; photoelectron spectroscopy, Zeeman Effect.

Prescribed Books

1. Banwell, C. N.; McCash, E. M.; Fundamentals of Molecular Spectroscopy, Tata McGraw-Hill, 4th edition, **2010**.
2. McQuarrie, D. A.; Simon, J. D.; Physical Chemistry: A Molecular Approach, University Science Books, **2011**.
3. Atkins, P. W.; Paula, J.; Physical Chemistry, Oxford Publications, 8th edition, **2009**.

Reference Books

1. Harris, D. C.; Bertolucci, M. D.; Symmetry and Spectroscopy: An Introduction to Vibrational and Electronic Spectroscopy, Dover Publications, **1989**.
2. Orchin, M.; Symmetry in Chemistry, John Wiley & Sons Inc., **2002**.
3. Levine, I. N.; Physical Chemistry, McGraw-Hill Science/Engineering/Math, 6th edition, **2008**.
4. Raff, L. M.; Principles of Physical Chemistry, Prentice Hall, **2001**.
5. I. N. Levine, Molecular Spectroscopy, John Wiley, **1975**.

Semester: 8**Subject Code: CHE0804****Credits: 4****4-1-0-4****Title: Physical Methods in Inorganic Chemistry**

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 – Evaluation of $10Dq$ and β for octahedral complexes of cobalt and nickel – applications to simple coordination compounds – charge transfer spectra – electronic spectra of $[\text{Ru}(\text{bipy})_3]^{2+}$.

Optical rotatory dispersion, circular dichroism and Magnetic circular dichroism – applications to metal complexes.

Infrared, Raman Spectroscopy and Mass Spectrometry: Vibrations in simple molecules (H_2O , CO_2) and their symmetry notation for molecular vibrations – 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 to inorganic compounds – Resonance Raman Spectroscopy.

Mass Spectrometry: Principles and presentation of spectra – molecular fragmentation – ion reactions – Inorganic applications.

NMR Spectroscopy

Examples for different spin systems – chemical shifts and coupling constants (spin-spin coupling) involving different nuclei (^1H , ^{19}F , ^{31}P , ^{13}C , ^{195}Pt) interpretation and applications to inorganic compounds – Effect of quadrupolar nuclei (^2H , ^{10}B , ^{13}B) on the ^1H 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.

EPR spectroscopy and Magnetic Properties

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.

Mossbauer Spectroscopy and NQR spectroscopy

Mossbauer 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.

ENDOR 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**.

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 Bioinorganic Chemistry*, John and Wiley & Sons, LTD, **2007**.
6. E. I. Solomon, A. B. P. Lever, *Inorganic Electronic Structure and Spectroscopy*, Vol., 2, Applications and Case Studies, Wiley-Interscience, **2006**.
7. A. B. P. Lever, *Inorganic Electronic Spectroscopy*, 2nd Sub Edition, Elsevier Science, **1986**.
8. D.N. Satyanarayana, *Electronic Absorption Spectroscopy*, Universities Press, **2000**.
9. R.B. Jordon, *Reaction Mechanisms of Inorganic and Organometallic Systems*, 3rd Edition, Oxford University Press, **2007**.
10. C.J. Ballhausen and H.B. Gray, *Molecular Orbital Theory*, Benjamin/Cummings Pub. Co, **1965**.
11. B. N. Figgis and M. A. Hitchman, *Ligand Field Theory and Its Applications*, 1st Edition, Wiley VCH, **1999**.
12. 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**.

Semester: 8

Subject Code: CHE0805

Credits: 3

0-1-5-3

Title: Advanced Inorganic Chemistry Laboratory

Estimation of copper, iron and nickel using spectrophotometry.

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°); the number of electrons transferred in the redox process (n); the diffusion coefficient (D); electrochemical reversibility; and the effects of varying concentration (C) and scan rate.
 2. Synthesis and study of $Mn^{III}(\text{Salen})\text{Cl}$ by Cyclic Voltammetry and Differential Pulse Voltammetry (DPV), and determination of the following: the formal reduction potential (E°); the number of electrons transferred in the redox process (n); the diffusion coefficient (D); electrochemical reversibility; and the effects of varying concentration (C) and scan rate.
 4. Preparation and determination of the effective magnetic moment and number of unpaired electrons in $Mn(\text{acac})_3$.
 5. Preparation and determination of the aquation rate of $[\text{Co}(\text{NH}_3)_5\text{Cl}]\text{Cl}_2$.
 6. Preparation and resolution of the optically active compound $[\text{Co}(\text{en})_3]^{3+}$.
 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

Reference Books

1. A. J. Elias, *A Collection of Interesting General Chemistry Experiments*, Universities Press, Sangam Books Ltd, **2002**.
2. J. D. Woollins, *Inorganic experiments*, 3rd Edition, Wiley-VCH Verlag GmbH & Co. KGaA, **2012**.
3. M. Hein, J. N. Peisen and R. L. Miner, *Foundations of College Chemistry in the Laboratory*, John Wiley and Sons, **2011**.
4. G. S. Girolami, T. B. Rauchfuss and R. J. Angelici, *Synthesis and Technique in Inorganic Chemistry: A Laboratory Manual*, 3rd Edition, University Science Books, **1999**.
5. W. L. Jolly, *The Synthesis and Characterization of Inorganic Compounds*, Prentice-Hall, Inc. **1970**.

Semester: 8

Subject Code: CHE0806

Credits: 3

0-1-5-3

Open ended Laboratory

Semester: 9

Subject Code: CHE0901

Credits: 4

4-1-0-4

Title: Main-Group and Organometallic Chemistry

Main group Organometallics: Classification and structure, ionic and electron deficient compounds of groups 1, 2 and 12.; Electron deficient compounds of the boron group; Electron-precise compounds of the carbon group. Electron-rich compounds of the nitrogen group. Low coordinate and hypervalent compounds – Relativistic effects on Chemical Reactivity.

Compounds with transition metal to carbon bonds: Classification of ligands, nomenclature, eighteen electron rule; transition metal carbonyls: range of compounds and structure, bonding, vibrational spectra, preparation, reactions; transition metal organometallics: square planar complexes, metal alkyls, metal alkylidenes and metal alkylidynes; Structure and bonding: metal-olefin bond and arene metal bond.

Compounds with ligands having extended pi systems: Bis(cyclopentadienyl) compounds, cyclopentadienyl carbonyl compounds, bis(arene) compounds, arene carbonyl compounds; isolobal analogy, metal-metal bond, transition metal clusters; clusters and catalysis; hydride and dihydrogen complexes; fluxionality.

Organometallic reactions and catalysis: oxidative addition, reductive elimination, insertion, hydride elimination, abstraction; olefin hydrogenation, hydroformylation, Wacker process, Ziegler-Natta polymerisation, cyclo oligomerisation, olefin isomerisation, olefin metathesis, Monsanto acetic acid synthesis, Fischer-Tropsch process, hydrosilylation.

Carbonylation, Hydrogenation, oxidation reactions, Isomerization reactions, Cross – coupling reactions, and CH functionalization reactions.

σ -Bonded ligands: Metal alkyls, aryls and hydrides. Stability, preparation and reactivity. Metal-carbonyls / Metal-phosphines / metal-nitrosyls / metal isocyanide: structures, reactivity and bonding. Metal-carbenes, metal-carbynes, Fischer carbenes, Schrock carbenes, N-heterocyclic carbenes, olefin metathesis.

π -Bonded ligands: Metal-olefins, metal alkynes, metal-dienes, Metal-Cp Metal-Cp* complexes. Synthesis, structure, bonding and reactivity.

Applications of organometallics in organic synthesis: C-C bond coupling reactions (Heck, Sonogoshira, Suzuki etc). C-N bond coupling reactions. Reduction reactions using transition metal hydrides; asymmetric hydrogenation.

Prescribed Books

1. P. Powell, *Principles of Organometallic Chemistry*, 2nd ed., Springer, **1998**.
2. K. F. Purcell and J. C. Kotz, *Inorganic Chemistry*, Saunders Golden Sunburst Series, W. B. Saunders Company, Philadelphia, **1977**.
3. 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**.

Reference Books

1. C. Elschenbroich and A. Salzer, *Organometallics: A Concise Introduction*, 3rd Edn. **1999**.
2. N. N. Greenwood and A. Earnshaw, *Chemistry of the Elements*, 2nd Edn., Elsevier, **2005**.
3. W. L. Jolly, *Modern Inorganic Chemistry*, McGraw Hill, New York, 2nd Edn., **1991**.
4. B. Douglas, D. McDaniel and J. Alexander, *Concepts and Models of Inorganic Chemistry*, John Wiley, New York, 3rd Edn., **1993**.
5. R. H. Crabtree, *Organometallic Chemistry of the Transition Metals*, Wiley, New York, **1988**.
6. S. E. Kegley and A. R. Pinhas, *Problems and Solutions in Organometallic Chemistry*, University Science Books, Oxford University Press.
7. A. J. Pearson, *Metalloorganic Chemistry*
8. A. W. Parkins and R. C. Poller, *An Introduction to Organometallic Chemistry*
9. I. Haiduc and J. J. Zuckerman, *Basic Organometallic Chemistry*
10. B. Douglas, D. H. McDaniel and J. J. Alexander, *Concepts and Models of Inorganic Chemistry*, 2nd ed, John Wiley & sons, New York.
11. Oxford Chemistry Primers Series, No. 12, M. Bochmann *Organometallics 1: Complexes with transition metal-carbon s bonds* and No. 13 M. Bochmann *Organometallics 2: Complexes with transition metal-carbon p-bonds*
12. J. P. Collman, L. S. Hegeudus, J. R. Norton and R. G. Finke, *Principles and Applications of Organotransition Metal Chemistry*, University Science Books. Mill Valley, California.
13. R. Hoffmann, *Angew. Chem. Int. Ed.*, Engl. 21, 711-800 **1982**.
14. BD Gupta and Anil J. Elias, *Basic Organometallic Chemistry: Concepts, Syntheses, and Applications of Transition Metals*, 1st edition, Universities Press, CRC Press, **2010**.

Semester: 9**Subject Code: CHE0902****Credits: 4****4-1-0-4****Title: Chemistry of biopolymers and natural products**

Carbohydrates: Classification, configuration of aldoses and ketoses, reactions of monosaccharides, chain elongation, chain shortening, stereochemistry of glucose, the Fischer projection, cyclic structure of mono saccharides, formation of glycosides, reducing and non-reducing sugar, determination of ring size, di-saccharides and poly-saccharides (Chemistry of maltose, starch and cellulose).

Amino acids, proteins and nucleic acids: Amino acids and proteins: Classification, preparation and stereochemistry of amino acids, isoelectric point, peptides, peptide synthesis, C and N- terminal analysis. Proteins - classification and primary, secondary and tertiary structure of proteins. Nucleic acids - Importance, classification, chemistry, purine and pyrimidine bases, chemical synthesis of nucleosides, nucleotides and nucleic acids. Structure of nucleic acids - protein synthesis- genetic code.

Steroids, bile acids and sex hormones: Chemistry, and structural elucidation of sterols and bile acids, estrogens, androgens, gestogens and adrenocortical hormones – biosynthesis of Cholesterol

Alkaloids: Occurrence, importance, general structural features, Hofmann exhaustive methylation, structure and synthesis of nicotine, piperine, quinine, and papaverine.

Vitamins: Chemical constitution and physiological functions of vitamins A, B2 (Riboflavin), C (Ascorbic acid)

Terpenes: Occurrence, isolation, classification, Isoprene rule, structure and synthesis of citral, geraniol and α -terpineol.

Reference Books:

1. I. L. Finar, *Organic Chemistry, Vol .2*, Fifth Edition
2. V. K. Ahluwalia, Lalita S. Kumar and Sanjiv Kumar, *Chemistry of Natural Products: Amino Acids, Peptides, Proteins, and Enzymes*, CRC press **2007**.
3. Sujata V. Bhat, *Chemistry of Natural Products*, Narosa, **2005**.
4. N R Krishnaswamy, *Chemistry of Natural Products: A Unified Approach*, Second Edition, CRC Press, **2010**.

Semester: 9

Subject Code: CHE0903

Credits: 4

4-1-0-4

Title: Advanced Thermodynamics

Review of the basics of thermodynamics, entropy and free energy concepts, reversible and irreversible processes

Fundamentals of open and closed systems, partial molar properties, Gibbs-Duhem equations, concepts of activity, fugacity.

Properties of gases, collision theory, the reaction co-ordinate & transition state, the formulation & decay of the activated complex, Eyring equation.

Boltzman factor and partition distribution, distribution of molecular states, configurations, molecular partition functions, applications

Statistical entropy, ensembles, canonical ensemble, Boltzmann distribution, Thermodynamic quantities and canonical partition function, Fermi-Dirac and Bose-Einstein distributions, molecular partition functions, translational, rotational and vibrational partition functions. Ideal monoatomic and diatomic gases.

Heat capacities-Einstein theory and Debye theories, classical partition functions, thermodynamic properties, equi partition theorem

Aspects of thermodynamics in equilibria, solutions and solids.

Debye-Huckel theory of strong electrolytes. Flory-Higgins theory of polymer solutions. Electrical conductivity of solutions, Butler-Volmer equation.

Theories of reaction rates- transition state theory, unimolecular reactions, reactions in solution, complex reactions including photochemical reactions and catalysis, reaction dynamics.

Irreversible processes and thermodynamics

Prescribed Books

1. McQuarrie, D. A.; Simon, J. D.; *Physical Chemistry: A Molecular Approach*, University Science Books, **2011**.
2. Atkins, P. W.; Paula, J.; *Physical Chemistry*, Oxford Publications, 8th edition, **2009**.
3. McQuarrie, D. A.; *Statistical mechanics*, University Science Publishers, **2000**.

Reference Books

1. Hill, T. A.; An Introduction to Statistical Thermodynamics, Dover Publications Inc., **1987**.
2. Levine, I. N.; Physical Chemistry, McGraw-Hill Science/Engineering/Math, 6th edition, **2008**.
3. Laidler, K. J.; Chemical Kinetics, Pearson Education, 3rd edition, **2011**.

Semester: 9**Subject Code: CHE0904****Credits: 3****0-5-1-3****Title: Advanced Organic Synthesis**

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 and Benzil – Benzilic acid rearrangements and Di- π -methane rearrangement.

Reagents in Organic Chemistry: Use of the reagents like Sodium borohydride, tri-n-butyl tin hydride, lithium dimethyl cuprate, lithium diisopropyl amide, trimethylsilyl iodide, diborane, ozone, CrO₃, DCC, DDQ, 9-BBN, lead tetra acetate, phenyl iodoso acetate, dimethyl sulphoxide, SeO₂, PCC, Yeast in organic synthesis and functional group transformations..

Phase transfer catalysis – benzyltriethylammonium halides- crown ethers.

Modern Synthetic methods: Baylis-Hillman reaction, Henry reaction, Nef reaction, Kulinkovich reaction, Ritter reaction, Sakura reaction, Tishcheko reaction and Ugi reaction, Brook rearrangement.

Metal mediated C-C and C-X coupling reactions Heck, Stille, Suzuki, Negishi, Sonogashira, Nozaki-Hiyama, Buchwald- Hartwig, Ullmann reactions and directed ortho-metalation.

Transition metal complexes in organic chemistry – homogeneous hydrogenation - Wilkinson's catalyst – umpoung synthesis.

Planning Organic Synthesis: An introduction to retrosynthesis - Synthons – 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.

Retro Diels – Alder reactions - Pericyclic reactions- Retrosynthesis of heterocycles containing two nitrogens.

Designing synthesis: Disconnection approach in natural products.

Green Chemistry: Principle, importance and applications.

Recommended Books:

1. F. A. Carey and R. A. Sundberg, Advanced Organic Chemistry, Part B: Reactions and Synthesis, Fifth edition, Springer, New York, **2007**.
2. W. Carruthers and I. Coldham, Modern methods of Organic Synthesis, First South Asian Edition, Cambridge University Press, **2005**.

3. J. March and M. B. Smith, March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure 6th Edition, Wiley, **2007**.
4. S. Warren, P. Wyatt, Organic Synthesis: The Disconnection Approach, Wiley, **2008**.
5. Organic Synthesis, Oxford Chemistry Primers, 31, C. L. Willis, M. Wills, Oxford Science Publications, **1996**.
6. Encyclopedia of Reagents for Organic Synthesis, 14 Volume Set, Leo A. Paquette, David Crich, Philip L. Fuchs, Gary A. Molander, Wiley, **2009**.
7. Workbook for Organic Synthesis: The Disconnection Approach, Stuart Warren, Paul Wyatt, Wiley, second edition, **2010**.
8. Introduction to Strategies for Organic Synthesis, Laurie S. Starkey, Wiley, **2012**.
9. Paul T. Anastas, Green Chemistry: Theory and Practice, Oxford University Press, USA, **2000**.

Semester: 9

Subject Code: CHE0905

Credits: 3

0-5-1-3

Title: Computational Chemistry Laboratory

Experiments involving optimization of molecular energies and geometries, calculation of thermodynamic parameters, kinetic parameters, prediction of spectral data.

Reference Books

1. J.B. Foresman, A Eleen Frisch, Exploring Chemistry with Electronic Structure Methods, Gaussian, Inc., 2nd Ed., **2000**
2. Frank Jensen, An Introduction to Computational Chemistry, John Wiley & Son Ltd., **1998**.
3. Christopher Cramer, Essentials of Computational Chemistry: Theories and Models, John Wiley & Sons, **2002**.

Semester: 9

Subject Code: CHE0906

Credits: 3

0-0-3-3

Title: Seminar and Literature Review

Students are required to take two seminars of one hour duration. 45 minutes presentation and 15 minutes of questions and discussion. Evaluation will be based on content of the material, presentation and depth of knowledge in the topic presented.

The student will be required to make a literature survey for the project that will be carried out in the subsequent semester assigned to a teacher. There won't be any external written examination.

Semester: 10

Subject Code: CHE1001

Credits: 9

0-3-12-9

Title: Research Project

Research project is carried out under the supervision of a teacher in the chosen field by the student. Normally it will be continuation of literature survey carried out from the yester semester.

Semester: 10 Subject Code: CHE10xx Credits: 3 2-1-0-3
 Title: Elective I

Semester: 10 Subject Code: CHE10xx Credits: 3 2-1-0-3
 Title: Elective II

Semester: 10 Subject Code: CHE10xx Credits: 3 2-1-0-3
 Title: Elective III

Semester: 10 Subject Code: CHE10xx Credits: 3 2-1-0-3
 Title: Elective IV

**List of Electives offered by the Department of Chemistry
 (Newer electives will be appended at the last)**

Course Code	Course Title
CHE1002	Chemistry of Nanomaterials
CHE1003	Carbohydrate Chemistry
CHE1004	Advanced Quantum Chemistry
CHE1005	Organocatalysis
CHE1006	Supramolecular Chemistry
CHE1007	Asymmetric Synthesis
CHE1008	Organic electronics
CHE1009	Biotransformations in Organic Chemistry
CHE1010	Advanced topics in organometallics
CHE1011	Advanced Techniques in Mass Spectrometry and NMR Spectroscopy
CHE1012	Principles of Polymer Chemistry
CHE1013	Introduction to Polymer Analysis
CHE1014	Medicinal Chemistry
CHE1015	Solar Cell Materials