SYLLABUS

M.Sc. (Chemical Sciences)

DEPARTMENT OF CHEMISTRY
PONDICHERRY UNIVERSITY
PONDICHERRY – 605 014

DEPARTMENT OF CHEMISTRY
PONDICHERRY UNIVERSITY

The Department of Chemistry belongs to the School of Physical, Chemical and Applied Sciences and it offers different programs leading to M. Sc. Integrated Program in Chemistry, M. Sc. Chemical Sciences, M. Phil. Chemistry and Ph.D. degrees. Students are admitted to M.Sc. Integrated program in Chemistry after 10+2 system of schooling, M.Sc. Chemical Science after three year under-graduation, M.Phil. Chemistry and Ph.D. after two year post-graduation. Details of eligibility criteria are available in the information brochure. Normally students are expected to take 10 semesters for M.Sc. Integrated program, 4 semesters for M.Sc. and 2/3 semesters for M.Phil. to complete requirements for the degree. The department follows Choice Based Credit System (CBCS). The students are expected to earn at least **192** credits for M.Sc. integrated program, **72** credits for M.Sc. and **36** credits for M.Phil. It is mandatory for the students to clear all the hard core courses and exercise selection from among the soft-core courses offered by the Department. Apart from the courses taken within the department, students are expected to take optional courses from among the breadth courses offered by sister departments in the University.

M.Sc. integrated and M.Sc. Chemcial Sciences students are expected to do project work spanning one semester in the final year. In addition, the students also do advanced practical. Both the advanced practical and the project courses are faculty oriented. Students are tuned to research in chemistry under the guidance of the selected faculty member.

The Department strives to provide broad based education in Chemistry at graduate, post-graduate and research levels. The students are expected to evolve interdisciplinary attitudes while going through various programs of the Department and the University.

M.Sc. Chemical Sciences

Course Structure

1st Semester

1. Inorganic Chemistry – I; CHEM 401; 3 credits; HC
2. Organic Chemistry- I; CHEM 421; 3 credits; HC
3. Physical Chemistry – I; CHEM 441; 3 credits; HC
4. Quantum Chemistry - I; CHEM 463; 3 credits; HC
5. Chemistry Lab – I ; CHEM 400; 3 credits; HC
6. Optional Course – I (to be taken outside the Department); 3 credits; SC

Number of Credits for the semester = 18

2nd Semester

1. Inorganic Chemistry – II; CHEM 402; 4 credits; HC
2. Organic Chemistry – II; CHEM 422; 4 credits; HC
3. Physical Chemistry – II; CHEM 442; 4 credits; HC
4. Quantum Chemistry - II; CHEM 464; 4 credits; HC
5. Chemistry Lab – II; CHEM 420; 3 credits; HC
6. Optional Course – II (outside the Department; 3 credits; SC)

Number of Credits for the semester = 22

3rd Semester

1. Inorganic Chemistry – III; CHEM 501; 4credits; HC
2. Organic Chemistry – III; CHEM 521; 4 credits; HC
3. Physical Chemistry – III; CHEM 541; 4 credits; HC
4. Spectroscopic Identification of Organic Compounds; CHEM 525; 3 credits; SC
5. Advanced Chemistry Lab; CHEM 500; (3 credits; HC)

Number of Credits for the semester = 18

4th Semester

1. Project and *viva* (CHEM 580; 5 credits; HC)
2. **Two** courses to be selected among the following:
    1. Inorganic Chemistry – IV; CHEM 502; 3 credits; SC
    2. Ligand Field Theory; CHEM 506; 3 credits; SC
    3. Inorganic Photochemistry; CHEM 504; 3 credits; SC
    4. Natural Products Chemistry; CHEM 524; 3 credits; SC
    5. Asymmetric Synthesis; CHEM 528; 3 credits; SC
    6. Magnetic Resonance Spectroscopy and Solid State Chemistry; CHEM 542; 3 credits; SC
    7. Magnetic Resonance; CHEM 544; 3 credits; SC
    8. Electro analytical Techniques; CHEM 546; 3 credits; SC
    9. Computational Quantum Chemistry; CHEM 562; 3 credits; SC
3. Optional Course – IV (outside the Department; 3 credits; SC)

Number of Credits for the semester = 14

TOTAL NO. OF CREDITS = 72

SYLLABUS

CHEM 400 LABORATORY COURSE IN CHEMISTRY – I

Pre-requisite: B. Sc. Degree; **HC**; **Credits: 3**

1. Preparation of Coordination Complexes using single step or multi step reactions.
2. Estimation of metal ions by complexometric and cerimetric titrations.
3. Semimicro qualitative analysis: Analysis of common and rare cations in a mixture.
4. EPR of inorganic ions and complexes.

CHEM 401 INORGANIC CHEMISTRY - I

Pre requisite: B. Sc. Degree; **HC**; **Credits: 3**

UNIT – I

Atomic Structure and Periodic Table: Atom as nucleus with orbital electrons, concept of wave-functions, quantum numbers and spin, shape of s, p and d orbitals and their radial distribution functions, electronic configuration of atoms, Aufbau principle, Pauli Exclusion Principle, and Hund's rule; Slater's rules for the determination of screening constants; arrangement of elements in Groups in the Periodic Table, s-block, p-block, d-block and f-block elements; periodic properties, ionic radii, ionization potential, electron affinity, electronegativity (Pauling, Mulliken and Aflred-Rochnow scales); atomic states and term symbols.

Bonding and structure: Types of bonds, ionic, covalent, coordinate, double and triple bonds; orbital symmetry and overlaps, concept of MO and VB theory, concept of hybridization, the extent of d orbital participation in molecular bonding; bond energy and covalent radii, concept of resonance, bond moment and molecular dipole moment; polarizing power and polarizability, Fajan's rules.

UNIT – II

Inorganic Solids and Nuclear Chemistry: Types of solids, covalent, ionic, molecular and metallic solids, lattice energy, cohesive energy and Medulong constants, Van der Waals forces, hydrogen bonding, unit cell, crystal lattices, structure of simple ionic compounds, z radius ratio and closed packed structures. Imperfections in crystals (point defects and F centers).

Nuclear chemistry: radioactive decay and equilibrium. nuclear reactions, Q value, cross sections, types of reactions, chemical effects of nuclear transformations; fission and fusion, fission products and fission yields; radioactive techniques, tracer technique, neutron activation analysis, counting techniques such as G. M. ionisation and proportional counter.

UNIT – III

Synthesis, properties and structures of Boron and Silicon compounds: Boron hydrides (small boranes and their anions, B_1–B_4), boron nitride, borazines, carboranes, metalloboranes, metallocarboranes; silicates, silicones, diamond, graphite, zeolites.

UNIT – IV

Nitrogen, Phosphorous, Sulphur and noble gas compounds: Hydrides, oxides and oxy acids of Nitrogen, Phosphorous, Sulphur and halogens; phosphazines, sulphur-nitrogen compounds, inter halogen compounds, pseudo halogens, noble gas compounds.

UNIT – V

Poly anions and isopoly anions of Phosphorous, Vanadium, Chromium, Molybdenum and Tungsten, heteropoly anions of Molybdenum and Tungsten; clathrates (noble gases, phosphazines) hydrogen bonding in clathrates, Phosphorous and Oxygen cage compounds.

Recommended Books:

1. J. E. Huheey, Inorganic Chemistry, Principles, Structure and Reactivity, Harper and Row, 3rd Edn, 1983.
2. N. N. Greenwood, A. Earnshaw, Chemistry of the Elements, 2nd Edn, Pergamon Press, 1989.
3. D. F. Shriver, P.W. Atkins, C.H. Langford, Inorganic Chemistry, 2nd Edn, ELBS, 1994.
4. W. L. Jolly, Modern Inorganic Chemistry, 2nd Edn., McGraw-Hill, 1991.
5. F. A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, A comprehensive Text, John Wiley, 5th Edn, 1987.
6. B. Douglas, D. McDaniel, J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Edn., John Wiley, 2001.
7. N. B. Hannay, Solid State Chemistry, Prentice Hall, New Delhi, 1976.
8. C. N. R. Rao and J.Gopalakrishnan, New Directions in Solid State Chemistry.
9. H. J. Arnikar, Essentials of Nuclear Chemistry, Wiley Eastern, 2nd Edn, 1988.

CHEM 421 ORGANIC CHEMISTRY – I
Pre requisites: B.Sc. Degree; **HC**; **Credits**: **3**

STRUCTURE BONDING AND REACTION MECHANISM.

UNIT – I
Structure bonding and introductory physical organic chemistry.
Review of structure and bonding in organic molecules: VB, MO and FMO theory.
Concept of hybridization, resonance, aromaticity, and anti-aromaticity.
Introductory physical organic chemistry – Acids and bases, HSAB, equilibrium constant; thermodynamic and kinetic effects; thermodynamic and kinetic control in organic reactions; Hammond postulate; Curtin-Hammett principle; Hammett equation.
UNIT – II
Stereochemistry and reactivity.
Review of basic principles of stereochemistry; configurational and conformational effects on reactivity; stereospecific and stereoselective reactions and diastereoselective reactions; chiral auxiliaries and asymmetric synthesis.
UNIT – III
Reactive intermediates.
Reactive carbon species – structure stability, formation and reactivity of carbanion, cabocation, radicals, carbene and benzynes.
Reactive heteroatom intermediates – structure, stability, generation and reactions of heteroatom electrophiles and nucleophiles.
UNIT – IV
Organic reaction mechanism – I.
Types and general mechanistic principles: Substitution at saturated and unsaturated reaction center (including aromatic compounds) by radical, nucleophile and electrophile; addition - elimination, elimination – addition mechanism
UNIT – V
Organic reaction mechanism –II
Addition reactions to carbon – carbon, carbon – heteroatom multiple bonds; isolated and conjugated multiple bonds. Elimination reactions: generating carbon – carbon and carbon – heteroatom multiple bonds.

Recommended books:
Adam Jacobs, Understanding organic reaction mechanism. Cambridge University press (1997).
M.A Fox and J.K. Whitesell., Organic chemistry, Jones and Bartlett Publishers (1994).
F.A. Carey and R. J. Sundberg (Part A and B) Kluwer Academic / Plenum Publishers (2000)
E,L.Eliel, Stereochemistry of carbon compounds. John Wiley (1997)
C.J. Moody and G.H. Whitham, Reactive intermediates Oxford chemistry Primers (1992).
S. Ege, Organic Chemistry, AITBS (2001)
Clayden et.al Advanced organic chemistry (2004)

CHEM 441 Physical Chemistry – I
Prerequisites: B.Sc. Degree; **HC**; **Credits: 3**

UNIT – I
Equilibrium Thermodynamics I
Concept of work and heat, first law of thermodynamics, enthalpy and heat capacities - concept of entropy, second law of thermodynamics, third law of thermodynamics-residual entropy.
UNIT – II
Equilibrium Thermodynamics II
Free energy, chemical potential, fugacity, liquids and solutions: ideal and non-ideal solutions, chemical equilibrium
UNIT – III
Statistical Thermodynamics I
BE, FD, MB statistics and distribution, ensembles, partition functions and molecular partition functions, mean energy
UNIT – IV
Statistical Thermodynamics II
Residual entropy, heat capacity of mono and diatomic gases, chemical equilibrium, Einstein and Debye theories of heat capacity of solids.
UNIT – V
Non-equilibrium thermodynamics
Postulates and methodologies, linear laws, Gibbs equation, Onsager reciprocal theory.

Recommended Books:
1. P. W. Atkins Physical Chemistry, 6th Edtion Oxford, 1998
2. L.A.Woodward,, Molecular Statistics, Oxford
3. Y. V. C. Rao, An Introduction to Thermo-dynamics, Wiley Eastern, 1993.
4. Physical Chemistry, R.S.Berry, S.A.Rice and J.Ross, Oxford, 2001.
5. M. Ladd, Introduction to Physical Chemistry, Cambridge, 1998.
6. D. A. McQuarrie and J. D. Simon,

Physical Chemistry, A molecular Approach, Viva, 1998.
7. F. W. Sears & G. L. Salinger, Thermodynamics, Kinetic Theory & Statistical Thermodynamics, Narosa, 1986.

CHEM 463: QUANTUM CHEMISTRY – I
Pre-requisites: B.Sc Degree in Chemistry with Maths at plus 2, CHEM 101 & CHEM 102; **HC**; **Credits: 3**

UNIT – I
Classical Mechanics and introduction to quantum mechanics
Lagrange's and Hamilton's equation of motion, Poisson Brackets. Inadequacy of classical mechanics, Schrodinger's and Heisenberg's formulation of quantum mechanics. Postulates .of quantum mechanics, need for operators, Linear and Hermitian operators, operator algebra, eigen value and eigen functions, commutation relations.
UNIT – II
Preliminary Mathematical Principles
Introduction to matrices, vector algebra, Differential equations, integrations in series. Legendre differential equations, Legendre and associated Legendre Polynomials, Hermite and Associated Laguerre polynomials. Orthogonal functions and Strum-Liouville problems.
UNIT – III
Wave Mechanics
Solution of Schrödinger's equation for the following systems-(I) particle in ID-, 2D- and 3D-boxes and applications, (2) particle in a ring and sphere, spherical harmonics, angular momentum rigid rotator, (3) Simple harmonic oscillator, and (4) Hydrogen atom. Zeeman effect and electron spin.
UNIT – IV
Approximate methods
Variation and Perturbation methods: examples: Variation methods: (1) Hydrogen atom, Hydrogen atom in an electric field, (2) Helium atom. Perturbation method: (1) perturbed particle in a box, (2) perturbed harmonic oscillator (3) Hydrogen atom in electric field.
UNIT – V
Atomic Structure
Antisymmetric wave functions of many electron atoms, Slater determinants, Hartree and Hartree-Fock self consistent field model for atoms. Electronic configuration of atoms, addition of angular momenta, spectroscopic term symbols, spin-orbit coupling, selection rules for atomic spectra.

Recommended books
1. S. N. Datta: Lectures on Chemical bonding and quantum chemistry, 1998.
2. D. A. McQuairrie: Quantum Chemistry, Oxford University press, Oxford, 1982.
3. P. W Atkins: Molecular Quantum Mechanics, Clarendon Press, Oxford, 1983.
4. R K. Prasad: Quantum Chemistry Through Problems and Solutions, New Age International, 1997.
5. Murre!, Kettle and Tedder:, Valency Theory, ELBS, London, 1966.
6. R. McWeeney: Coulson's valence, Oxford-ELBS (3rd ed.) 1976.
7. Karplus and Porter: Atoms and molecule, 1973.
8. F. L. Pilar: Elementary quantum chemistry, Mc-Graw Hill International, 2nd ed. 1990.
9. A. K Chandra: Introduction to Quantum Chemistry, Tata McGraw Hill, 1988.
10. E. Kreyzig; Advanced Engineering Mathematics.
11. Goldstein: Classical Mechanics

CHEM 420 LABORATORY COURSE IN CHEMISTRY – II
Pre-requisites: B.Sc. Degree; **HC**; **Credits 3**

1. Introductory experiments on chromatographic techniques – TLC, CC and PC
2. Preparation of organic compounds by one or two steps.
3. Separation and identification of two or more organic compounds in a mixture.
4. Experiments in physical chemistry involving electrochemistry and the use of computers in analyzing data. Use of packages like ORIGIN and MATHEMATICA

   Recommended books: Vogel's Text Book of Practical Organic Chemistry

CHEM 402 INORGANIC CHEMISTRY - II
Pre requisites: B.Sc. Degree; **HC**; **Credits: 4**

UNIT – I

Introduction to transition metal complexes: Brief review of the general characteristics of transition elements, types of ligands, nomenclature of coordination complexes, chelates, chelate effect, geometry and isomerism, formation of complexes, stability constants, Werner, Sidzwick and VSEPR theory.

UNIT – II

Electronic structure of transition metal complexes 1:

Crystal field theory, crystal field splitting, application of d-orbital splittings to explain magnetic properties, low spin and high spin complexes, crystal field stabilization energy, spectrochemical series, weak and strong field complexes, thermodynamic and related aspects of crystal fields, ionic radii, heats of ligation, lattice energies, site preference energies.

UNIT – III

Electronic structure of transition metal complexes 2:

VB and MO theory of complexes (quantitative principles involved in complexes with no pi and with pi bonding) and ligand filed theories and molecular symmetry, angular overlap model, Jahn Teller effect, electronic spectra of transition metal complexes, orgal and Tanabe-Sugano diagrams, charge transfer and d-d transitions, nephelauxetic series.

UNIT – IV

Inorganic reaction mechanisms: inert and labile compounds, substitution reactions of octahedral complexes, dissociative, associative, anation, aquation, conjugate base mechanism; substitution reactions of square planar complexes, trans effect, trans effect series, theories of trans effect; electron transfer reactions.

UNIT – V

Magnetism: dia, para, ferro and antiferro magnetism, quenching of orbital angular moment, spin orbit coupling; Chemistry of lanthanides and actinides: lanthanide contraction, oxidation states, spectral and magnetic properties, use of lanthanide compounds as shift reagents.

Recommended Books:

1. F. A. Cotton, G. Wilkinson, Advanced Inorganic Chemistry, 5th Edn., John Wiley.
2. J. E. Huheey, Inorganic Chemistry, 3rd Edn., Harper International, 1983.
3. B. Douglas, D. McDaniel, J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Edn., John Wiley, 2001.
4. D. F. Shriver, P. W. Atkins, C. H. Langford, Inorganic Chemistry, ELBS. 1990.
5. N. N. Greenwood, A. Earnshaw, Chemistry of the Elements, 2nd Edn., BH, 1997.
6. W. L. Jolly, Modern Inorganic Chemistry, 2nd Edn., McGraw-Hill, 1991.
7. J. D. Lee, A New Concise Inorganic Chemistry, 3rd Edn., ELBS, 1987.

CHEM: 422; ORGANIC CHEMISTRY – II

Pre requisites: B. Sc. Degree; **HC**; **Credits**: **4**

Heterocyclic Chemistry and Bioorganic Chemistry.

Unit – I

Heterocyclic chemistry - I.

Nomenclature, Non-aromatic heterocyclic compounds – three, four, five, six member rings with one hetero atom (N, O, S) , structure, synthesis and reactions.

Unit – II

Heterocyclic chemistry – II.

Aromatic heterocyclic compounds – five and six membered heterocyclic systems with one and two hetero atoms (N, O, S) . Benzo fused heterocyclic systems – Indole, Quinoline, Isoquinoline - structure, synthesis and reactivity.

Unit – III

Biomolecules -I

Lipids and Carbohydrates.

Lipids: Fats and Waxes, Miscelles, Bilayer membranes.

Carbohydrates – mono, di, and polysaccharides – Structure of representative examples.

Unit – IV

Biomolecules –II.

Aminoacids, peptides, proteins – structure and synthesis including solid phase synthesis.

Unit – V

Biomolecules – III.

Nucleic acids and nucleotides – structure and biochemistry.

Recommended Books:

T.L.Gilchrist, Heterocyclic Chemistry. John Wiley & Sons, (1987).

J.A Joule and K.Mills, Heterocyclic Chemistry, Fourth edition, Blackwell Science Ltd, (2000).

E.E Conn, P.K Stumpf and Doi, Biochemistry, John Wiley , (1992).

CHEM 442 – PHYSICAL CHEMISTRY - II

Pre-requisites: B.Sc. Degree; **HC**; **Credits: 4**

UNIT – I

Basic Chemical Kinetics

Molecularity, order and rate of reactions, Arrehenius theory - Complex reactions: reversible, pre-equilibrium, consecutive, chain and photochemical, oscillatory reactions, enzyme kinetics - Lindenmann's theory of uni-molecular reactions - laser flash photolysis, flow techniques and relaxation methods

UNIT – II

Molecular reaction dynamics

collision and activated complex theory, comparison of results with Eyring and Arrhenius equations - reactive collisions, molecular beam experiments, introduction to potential energy surfaces: treatment of H_2 + H reaction - ionic reactions: salt effect

UNIT – III

Surface phenomena

Growth and structure of surface, surface defects, kinetics of surface adsorption: Langmuir and BET isotherms.

UNIT – IV

Equilibrium electrochemistry

Activities in electrolytic solutions, mean activity coefficient, Debye-Huckel treatment of dilute electrolyte solutions, origin of electrode potential, half cell potential, electrochemical cell, Nernst equation, thermodynamics of electrochemical cell

UNIT – V

Dynamic electrochemistry

Electrical double layer - electrode kinetics: rate of charge transfer, current density, Butler- Volmer equation - introduction to polarography, cyclic voltammetry - theory of corrosion and inhibition of corrosion - fuel cells.

Recommended Books:

1. K. J. Laidler, Chemical Kinetics, 3rd Edn., Harper International, 1987.
2. G. L. Agarawal, Basic Chemical Kinetics, Tata McGraw Hill, 1990.
3. G. D. Billing & K. V. Mikkelson, Molecular Dynamics and Chemical Kinetics, John Wiley, 1996.
4. J. I. Sheinfield, J. S. Francisco, W. L. Hasse, Chemical Kinetics & dynamics, Prientice Hall, 1998.
5. A. J. Bard & L. R. Faulkner, Electro-chemical Methods, Fundamental and Applications, John Wiley, 1980.
6. Bockris & Reddy, Electrochemistry, Vol. 1& 2, Plenum, 1973
7. P. H. Reiger, Electrochemistry, Prentice Hall, 1987.
8. H. V. Keer Solid State Chemistry, Wiley Eastern, 1993.
9. A. K. Cheetam & P. Day, Solid State Chemistry Techniques, Oxford, 1987.

CHEM 464 QUANTUM CHEMISTRY - II

Pre-requisites: B.Sc Degree in Chemistry with Maths. at plus 2, CHEM 101 & CHEM 102; **HC**; **Credits: 4**

UNIT - I

Group Theory any Symmetry-I

Axioms and theories of group- sub-groups-classes. Molecular symmetry and point groups: Symmetry elements and operators, classes of symmetry operation, Symmetry classification of molecules. Matrix representation of symmetry operations, representation of groups, character, reducible and irreducible representations. Double groups. 9L

UNIT - II

Group Theory and Symmetry -II

Great Orthogonality theorem, Character tables, symmetry properties of Hamiltonian operator, wave functions as basis for irreducible representations. Transition moment integrals, selection rule for spectral transitions. Mutual exclusion principle, Projection operators and construction of symmetry adopted linear combinations. 9L

UNIT – III

MO and VB theory of Diatomic Molecules

Simple Mo theory for homo and heteronuclear diatomics, non-crossing rule, correlation diagrams for homo and heeronuclear diatomics, MO configuration for diatomics, dipole moments of homo nuclear diatomic molecules.

VB theory: Heitler-London Wavefunction for hydrogen molecule, Q and J integrals, Covalent and ionic structures, singlets and triplets. Defects in the simple MO and VB theories, electron correlation problem, configuration interaction, equivalence of MO and VB theories, Coulson-Fischer function, hybridization in LiB and CO. 9L

UNIT - IV
Polyatomic Molecules
Polyatomic Molecules- localized and delocalized molecular orbitals, H2O molecule, hybridization and non-equivalent hybrids, construction of sp, Sp^2, Sp^3, dsp^2, and d^2sp^3 hybrids and non-equivalent sp, Sp^2, and Sp^3 hybrids. 9L

UNIT - V
Huckel and SCF Theories
Simple Huckel theory for p-electrons, Frontier orbitals, Extended Huckel theory. Advanced MO methods: SCF theory for molecules, Slater determinants, electron repulsion integrals. Roothan' s equation. ZDO approximations, PPP, CNDO and INDO approximations. Hellman-Feynman theorem: some simple applications (qualitative treatment only). 9L

Recommended Books

1. F. A. Cotton: Chemical Applications of Group Theory, Wiley Eastern, 1985.
2. P. K Ghosh and P. K Shukla:Atomic Electronic Structure, Prentice Hall ofIndia,1994.
3. v. Ramakrishnan and M. S. Gopinathan: Group Theory in chemistry, Vishal Publication, 1986.
4. I. N. Levine: Quantum Chemistry, Prentice Hall India, 1994.
5. S. N. Datta: Lecture on Chemical bonding and quantum chemistry, 1998.
6. D. A. McQuairrie: Quantum Chemistry, Oxford University press, Oxford,1982.
7. P. W Atkins:. Molecular Quantum Mechanics, Clarendon Press, Oxford, 1983.
8. R. K. Prasad: Quantum Chemistry through Problems and Solutions, New Age International, 1997.
9. Murrel, Kettle and Tedder: Valency Theory, ELBS, London, 1966.
10. R. McWeeney: Coulson's valence, Oxford-ELBS(3rd ed.) 1976.
11. Kaplus and Porter: Atoms and molecule, 1973.
12. F. L. Pilar: Elementary quantum chemistry, Mc-Graw Hill International, 2nd ed. 1990.
13. A. K Chandra: Introduction to Quantum Chemistry, Tata McGraw Hill, 1988.

CHEM 500 ADVANCED LABORATORY COURSE IN CHEMISTRY
Pre-requisite: Consent of teacher; **HC**; **Credits: 3**

Students are allotted to various faculties of the department. They will be working under the supervision of the respective faculties.

CHEM 501 INORGANIC CHEMISTRY – III
Pre requisites: B.Sc. Degree; **HC**; **Credits: 4**

UNIT – I
Organometallic Chemistry 1:
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.

UNIT – II
Organometallic Chemistry 2:
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.

UNIT – III
Organometallic Chemistry 3:
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.

UNIT – IV
Bioinorganic Chemistry 1:
Metal ions in biological systems: heme proteins, hemoglobin, myoglobin, hemerythrin, hemocyanin, ferritin, transferrin, cytochromes and vitamin B12; Iron-sulphur proteins: rubredoxin, ferredoxin and model systems.

UNIT – V
Bioinorganic Chemistry 2:
Metalloenzymes: active sites, carboxy

peptidase, carbonic anhydrase, superoxide dimutase, xanthine oxidase, peroxidase and catalase; photosynthesis, water oxidation, nitrogen fixation, nitrogenase; ion pump, metallodrugs.

Recommended Books:

1. P. Powell, Principles of Organometallic Chemistry, 2nd Edn., ELBS, 1991.
2. J. E. Huheey, Inorganic Chemistry, 3rd Edn., Harper International, 1983.
3. C. Elschenbroich, A. Salzer, 2nd Edn., VCH, 1992.
4. M. F. Purcell, J. C. Kotz, Inorganic Chemistry, Saunder, 1977.
5. F. A. Cotton, G. Wilkinson, Advanced Inorganic Chemistry, 5th Edn., John Wiley.
6. R. W. Hay, Bio Inorganic Chemistry, Ellis Horwood, 1987.
7. R. M. Roat-Malone, Bio Inorganic Chemistry, John Wiley, 2002.
8. T. M. Loehr, Iron carriers and Iron proteins, VCH, 1989.
9. S. J. Lippord, Progress in Inorganic Chemistry, John Wiley, Vol. 30, 1983.

CHEM 521 - ORGANIC CHEMISTRY – III
Prerequisite: CHEM 421; **HC**; **Credits: 4**

UNIT – I
Concerted Reactions
Mechanism and synthetic applications of cycloaddition, electrocyclic, sigmatropic and related pericyclic reactions. Explanation based on frontier orbital, correlation diagram and Huckel-Mobius approachs.
UNIT – II
Organic Photochemistry:
Introduction – Frank-Condon principle – Jablonski diagram – Basic organic photochemical reactions involving alkenes, arenas, carbonyl and azide functional groups. Remote fictionalization. Application of photochemical reactions in organic synthesis.
UNIT– III
Rearrangement Reactions
Rearrangement of organic molecules and their synthetic potential; Rearrangement reactions involving carbo-cations, carbene, carbanion, and nitrene intermediates.
UNIT – IV
Oxidation and Reduction Reactions
Oxidation of organic compounds with reagents based on peroxides, peracids, ozone, osmium, chromium, ruthenium, silver, dimethyl sulfoxide iodine, and selenium dioxide. Reduction of organic compounds with reagents based on boron, aluminum, hydrogen, hydrazine, formic acid and dissolving metals.
UNIT – V
Modern Reagents in Organic Synthesis
Introductory treatment to the application of silicon, boron (organo boranes), phosphorus, palladium, samarium, ruthenium, indium reagents in organic synthesis.

1. J.D. Coyle, Organic Photochemistry - Wiley, 1985.
2. Carruthers, Modern Methods in Organic Synthesis, Academic Press, 1989.
3. F. A. Carey and R. Sundberg, Advanced Organic Chemistry, Vol. 1 and 2 (2002)

CHEM 541 PHYSICAL CHEMISTRY - III
Pre-requisite: B.Sc. Chem.; **HC**; **Credits: 4**

Unit – I
Microwave and IR spectroscopy:
Electromagnetic radiation, interaction of electromagnetic radiation with matter, quantum mechanical approach - transition probabilities: Einstein coefficients - pure vibrational and rotational spectra, selection rules, vibrational and rotational spectra of polyatomic molecules, normal modes, anharmonicity, selection rules - Raman effect: classical and quantum theory of Raman effect, rotational and vib-rotational Raman spectra
UNIT – II
Electronic spectroscopy
Transition moments, assignment of electronic transitions of N_2, H_2O and formaldehyde using group theory, fluorescence and phosphorescence, ESCA, PES, AUGER techniques
UNIT – III
Magnetic Resonance I: introduction to nmr
Origin of magnetic moments in matter, electronic and nuclear moments, interaction with magnetic field, Larmor equation - conditions for magnetic resonance absorption, relaxation times, line widths and line shapes, chemical shifts, ring currents, diamagnetic anisotropy, spin-spin splitting, high resolution NMR spectra of simple molecules, first and second order treatment of AB systems - FT techniques

UNIT – IV
Magnetic Resonance II: EPR, NQR and mossbauer spectroscopic techniques
Electron spin resonance: g value, hyperfine structure, esr of organic free radicals, esr of solids, esr of inorganic ions, esr of simple free radicals in solutions - NQR and Mossbauer spectroscopy.

UNIT – V
Introductory solid state chemistry: .
Crystal morphology, Mi1ler indices - x-ray diffraction - close packing, factors affecting crystal structure, defects, vacancies and dislocations - LEED, neutron diffraction and electron diffraction.

Recommended Books:

1. P. W. Atkins, Physical Chemistry, Oxford, London, 6th edition, 1998.
2. R. Sindhu, Molecular Spectroscopy, Tata McGraw Hill, 1986.
3. Banwell, Molecular Spectroscopy, Tata McGraw Hill, 1998.
4. A. Carrington and Machlachlon, Magnetic Resonance, Harper & Row, 1967.
5. Graebeal, Molecular Spectroscopy, Prientice Hall, 1968.
6. G. M. Barrow, Introduction to Molecular Spectroscopy, McGraw Hill, 1964.

CHEM 525 SPECTROSCOPIC IDENTIFICATION OF ORGANIC COMPOUNDS.
Pre requisites: B.Sc. Degree; **SC Credits: 3**

UNIT – I
Introduction to spectroscopic techniques of structure elucidation and Application of UV – Visible and IR spectroscopy to organic structure elucidation.
Electromagnetic radiation, energy and electromagnetic spectrum, units, absorption of energy by organic compounds, types of spectroscopic methods to organic structure elucidation.
UV – Visible Spectroscopy: Basic principles, application of UV – Visible spectroscopy to organic structure elucidation, Woodward – Fisher rules, Octant rule, Application of ORD – CD to stereochemical assignments.
IR – Spectroscopy – Basic principles, characteristic frequencies of common functional groups.

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

UNIT – III
Multinuclear NMR (with specific emphasis on 13-C NMR)
13C NMR: Proton coupled, off–resonance decoupled, proton noise decoupled 13C NMR spetra. Assignment of chemical shifts, additively effect, characteristic chemical shifts of common organic compounds and functional groups, DEPT and SEFT spectra. Introduction to multinuclear NMR of common hetero atoms present in organic compounds (N, F, O, P S & D). 2D NMR techniques 1H – 1H COSY, 1H – 13C COSY – HMBC, NOESY and INADEQUATE spectra.

UNIT – IV
Application of mass spectroscopy to organic structure elucidation.
Basic principles, techniques of ion production and ion and daughter ions, molecular ion and isotope abundance, nitrogen rule energetics of fragmentation ,
Metastable ions, common fragmentation pathways – fragmentation pattern of common chemical classes.

UNIT – V
Problem solving excercises involving UV, IR NMR & MS data

Recommended books:

William Kemp, Organic Spectroscopy, Third Edition , MacMillon (1994).
D.H Williams and Ian Fleming, Spectroscopic methods in organic chemistry, Tata McGraw Hill, (1998).
R.M. Silverstein and F. X. Webster, Spectrometric identification of organic compounds; John Wiley and Sons. Inc., Sixth edition (1997).
William Kemp, Introduction to multinuclear NMR.

CHEM 502 INORGANIC CHEMISTRY – IV
Pre-requisite: B.Sc. Degree; **SC Credits: 3**

UNIT – I
Concepts of Supramolecular Chemistry: Definition, Nature of supramolecular interactions, Host-guest interaction, Molecular recognition, Types of recognition,

Self-assembly.

UNIT– II

Cation-binding Hosts:

Concepts, Cation receptors, Crown ethers, Cryptands, Spherands, Calixarens, Selectivity of cation complexation, Macrocyclic and template effects.

UNIT – III

Binding of Anions and Neutral molecules:

Concepts, Anion host design, Anion receptors, Shape and selectivity, Neutral receptors, clathrates, cavitands, cyclodextrins, cyclophanes.

UNIT – IV

Applications of Supramolecular Chemistry:

Rational Design, Molecular Paneling, Supramolecular reactivity and catalysis, Supramolecular devices, Nanoscience applications.

UNIT – V

Supramolecular Chemistry in Biology:

Membranes, Macrocyclic systems, Photosynthesis, Oxygen transport, Biological mimics, Enzymes, Metallobiosites, Heme analogues.

Recommended Books:

1. J. M. Lehn, Supramolecular Chemistry, Concepts and Perspectives, VCH, 1995.
2. H. Dodziuk, Introduction to Supramolecular Chemistry, Kluwer Academic, 2002.
3. F. Vogtle, Supramolecular Chemistry, An Introduction, John Wiley & Sons, 1991.
4. J. W. Steed, J. L. Atwood, Supramolecular Chemistry, A Concise Introduction, John Wiley, 2000.
5. A. Bianchi, K. B. James, E. G. Espana, Supramolecular Chemistry of Anions, Wiley-VCH, 1997.
6. M. Fujita, Molecular Self-assembly, Organic Versus Inorganic Approaches, Springer, 2000.
7. J. L. Atwood, J. E. D. Davies, D. D. MacNicol, F. Vogtle, J. M. Lehn, Comprehensive Supramolecular Chemistry, Pergamon, 1996.

CHEM 504 INORGANIC PHOTOCHEMISTRY

Pre-requisite: CHEM 402, CHEM 501, **SC**

Credits: 3

UNIT – I

Basic principles:

Absorption of light –photochemical laws – photostationary states – rate law – photolysis – quantum yields – actinometry – scavenging of reaction intermediates – flash photolysis – single photon techniques – flow techniques – picosecond transient kinetics.

UNIT – II

Kinetics of photoluminescence:

Thermal effects of photoluminescence – luminescence yield – time resolved detection of excited states – radiative and non radiative transitions – energy transfer.

UNIT – III

Photoredox reactions:

Charge transfer complex – theory of electron transfer reactions – reactivity of CTTM, CTTL excited states – medium effects

UNIT – IV

Ligand field photochemistry:

General features of ligand field photochemistry – reaction of excited states of d^n metal complexes.

UNIT – V

Organometallic photochemistry:

Excited states in organometallic compounds – metal carbonyls – compounds with □ or □ M – C bonds – hydride complexes.

Recommended Books:

1. K.K. Rohatgi-Mukherjee, Fundamentals of Photochemistry, Tata-McGraw Hill, 1981.
2. J. Calvert and J.N. Pitts, Photochemistry
3. Collected readings in inorganic photochemistry, J. Chem. Edn. 1983
4. G. J. Ferraudi, Inorganic photochemistry, 1973
5. A.W. Adamson, E.D. Fleishcer, Concepts in inorganic photochemistry, 1963

CHEM 506 LIGAND FIELD THEORY

Pre-requisites: CHEM 463 &CHEM 464, **SC**

Credits: 3

UNIT – I

Introduction:

Qualitative basis of crystal fields, Atomic spectroscopy (free ion, free ion terms, term wave functions, spin-orbit coupling), Thermodynamic aspects of crystal fields.

UNIT – II

Ions in Crystal Field:

Free ions in weak crystal fields (effect of a cubic crystal field on S,P,D,F,G,H, and I terms), Free ions in Medium and strong

crystal fields.
UNIT – III
MO theory of complex ions:
Bonding in O_h/T_d complexes, qualitative calculations of 10Dq, Electronic spectra of complex ions.
UNIT – IV
Magnetic properties of complex ions:
Complexes of non-cube stereochemistry, Actinide element compounds
UNIT – V
ESR of complex ions:
Theory and evaluation of spin Hamiltonian parameters for systems with s=1/2 and s >1/2.

Recommended Books:

1. B.N. Figgis, Introduction to Ligand Fields, Wiley Eastern Ltd., New Delhi/Bangalore, 1976.
2. A. B. P. Lever, Inorganic Electronic Spectroscopy, Elsevier, 1986.

CHEM 524 NATURAL PRODUCTS CHEMISTRY
Pre-requisite: CHEM 422; **SC**; **Credits: 3**

UNIT – I
Chemistry of Terpenes:
Biosynthesis of acyclic and monocyclic terpenes from acetyl CoA; synthesis of *trans* chrysanthemic acid; biosynthesis of loganin and seco-loganin; asymmetric synthesis using limonene and menthol; chenmical degredation, structure and synthsis of alpha-pinene and camphor; biosynthesis of sesquiterpenes; structure, transannular cyclisation and synthesis of caryophyllene; FVP route to corriolin and hirsutene; structure and synthesis of iswarane and longifolene – 10 lectures.
UNIT – II
Biosynthesis of diterpenes; structure and synthesis of podocarpic acid, abietic acid and kaurene; introductions to gibberellic acids, synthesis of gibberillic acid A3; structure, synthesis and biological activity of paclitaxel; introduction to gincolides, biosynthesis of squalene; cyclization of squalene epoxide; structures of representative examples of higher terpenes, quassin, beta-amyrin, cucubitacine etc. – 10 lectures
UNIT – III
Steroids and polyphenolics:
Biosynthesis of Steroids - Structure of common steroids such as cholesterol, ergosterol, stegmasterol, vitamin D, Cholic acid; Steroidal hormones estrone, progesterone, aldostrone, testosterone; synthetic approaches towards steroids (both laboratory and industrial).
Introduction to flavones, isoflavones, anthocyanins and aurones – 10 lectrures
UNIT – IV
Alkaloids and Antibiotics:
Classification of alkaloids based on biosynthesis; Biosynthesis of tyrosine, tryptophan; structure determination and synthesis of nicotine, morphine, cocaine, yohimbine, reserpine, strychnine and quinine; Structure and synthesis of beta-lactam antibiotics (penicillin and cephalosporin) and tetracylic antibiotics - 15 lectures
UNIT – V
Introduction to Marine Natural Products - 5 lectures

Recommended Books:

1. K. Nakanishi, Natural Product Chemistry Blackie Publications, Vols I, II, III.
2. R.H. Thomson, Chemistry of Natural Products - Wiley, New York, 1996.
3. I.L. Finar, Advanced Organic Chemistry, Vol. 2 ELBS, New Delhi, 1975.

CHEM 528 ASYMMETRIC SYNTHESIS
Prerequisites: CHEM 421; CHEM 422 and CHEM 521; **SC**; **Credits: 3**

UNIT – I. Introduction to asymmetric synthesis:
Basic principles of Asymmetric synthesis – Definition - Stereospecific, Stereoselective – enanatioselective and diastereoselective. Importance of asymmetric synthesis, conditions for an efficient asymmetric synthesis, energetic considerations, strategies for asymmetric synthesis-advantages and limitations of each strategy, analytical methods for determining enantiomeric excess. Resolving agents and resolution of racemic compounds having common functional groups for eg. alcohol, amine, acid. Resolution of chiral ligands - BINOL, *trans* 1,2-diaminocyclohexane. Interaction between chiral substrate and chiral reagent. Kinetic resolution of racemic mixtures.
UNIT – II Asymmetric synthesis on chiral substrate:
Nucleophilic addition to α–chiral carbonyl compounds; Prediction of stereochemistry-

Cram's rule and related modifications. Double stereo differentiation; matched pair and mismatched pair; examples from aldol condensation and hydroboration reactions. Electrophilic addition to α – chiral olefins - epoxidation, cyclopropanation, hydroboration – oxidation, alkylation of enolates of β-chiral carbonyl compounds.

UNIT – III Asymmetric synthesis using chiral reagents

Chiral organo boranes -Application of chiral organoboranes, reduction (Ipc_2BCl) and allylation and crotylation reactions, T.S models; Chiral modification of lithium aluminum hydride, BINAL-H - application in reduction of prochiral ketones; oxazaborolidines. T.S model; Asymetric Michael addition to α ,β – unsaturated carbonyl compounds T.S model; chiral lithium amides – enantioselective deprotonation.

UNIT – IV Asymmetric synthesis using chiral auxiliary:

Chiral auxiliaries derived from proline, champhor, menthol and other chiral pool sources. SAMP / RAMP hydrazines, and other pyrrolidines, oxithiane, oxazolidine-2-one, thiazolidine-2-one, phenylethylamine, 2-phenylcyclohexanol, 8-phenyl menthol.

UNIT – V Asymmetric synthesis using chiral catalysts:

Asymmetric alkylation and allylation of carbonyl compounds, chirality amplification, non-linear effects: Selected reactions: DAIB, Keck's allylation, TADDOLs and other privileged ligands. Asymmetric hydrogenation: early advances DIPAMP, DIOP and Noyori's BINAP - selected reactions / examples. Proline mediated aldol reactions and further expansion in the field of organo catalysis. Sharpless epoxidation, dihydroxylation, aminohydroxylation of alkenes; Utility metal-semicorrinato complexes and Jacobson catalysts – Evans catalyst - Aziridination.

Books for reading and reference

Asymmetric Synthesis: Morrison, J. D. Vol 1-5, Academic press, 1983.
Stereochemsitry of Carbon compounds: E. L. Eliel, Wiley, 1992.
Comprehensive Asymmetric Catalysis (Jacobsen, E. N,; Pfaltz, A. Yamamoto, H. Eds.) Springer 2000.
Asymmetric Catalysis in Organic synthesis: Noyori, R. Wiley-NY 1994.
Catalytic Asymmetric Synthesis: Ojima, I. VCH-NY, Pergamon, 1998.
Methods for the Asymmetric Synthesis of Complex Organic Molecules, Daniel J. O'Leary, Lecture Notes 2001.
Principles of Asymmetric Synthesis (Tetrahedron series in Organic Chemistry), R. E. Gawley, J Aube, Pergman, 1996
Aymmetric Synthesis, H. B. Kagan, Thieme Medical Publishers, I[st] Edn., 2003.
Asymmetric Synthesis, G. Proctor, Oxford University Press, USA, 1997.

CHEM 542: MAGNETIC RESONANCE SPECTROSCOPY & SOLID STATE CHEMISTRY

Pre-requisite: CHEM 401; **SC**; **Credits: 3**

UNIT – I

Magnetic Resonance-I

Classical and quantum mechanical description of resonance, Bloch's equations and solution for a weak rf-field, complex susceptibilities, nuclear induction, FT techniques, 900and 1800 pulses, spin echoes, measurements of T 1 and T 2 by pulse techniques, NOE, 2D-J-resolved NMR, COSY.

UNIT – II

Magnetic Resonance-II

Spin-Hamiltonian for hydrogen atom, first and second order perturbation treatment, isotropic and anisotropic hyperfine interactions. Mechanism of hyperfine interactions in aromatic radical ions in solutions, spin density, McConnel relation. EPR in solids: g- and A- matrices, effective spin Hamiltonian, treatment for p1 and dl ions. Single crystal and powder EPR lineshapes, S >1/2 systems with emphasis on zero-field splitting. }

UNIT – III

Solid State Chemistry-I

Imperfactions and related phenomena- Defects in Solids: Point defects, line defects and plane defects. Thermal properties- Heat capacities of Solids: Dulong-Petit law, Einstein and Debye theories, thermal conductivity of insulators and thermal expansion coefficient. Electrical conductivity- origin of band gap, Fermy energy, density of states, thermal conductivity of metals, semiconductors and superconductivity.

UNIT – IV

Solid State Chemistry-II

Magnetic properties: classification of magnetic materials, quantum mechanical theory of paramagnetism, nuclear paramagnetism, ferro- antiferro- and ferrimagnetism. Solid state transformations, solid state reactions, theory and techniques of crystal growth.

UNIT – V

Solid State Chemistry-III

Diffusion in solids: diffusion mechanisms, Ficks laws of diffusion, diffusion as a random walk problem. Optical properties: thermionic emmission, photovoltaic effect, optical absorption of semiconductors. Dielectric properties: dielectric constant and related properties, behaviour of dielectric materials in ac fields, Clausius-mosotti equation. Thermoelectric effects: Thompson effects, peltier effect, seebeck effect, thermocouples and Hall rffect. Hopping semiconductors, polarons , liquid crystals, and glasses. Pauling's rules in polyhedral structural chemistry

Recommended Books

1. H. V. Keer, Principles of Solid State, Wiley Eastern Limited, 1993
2. W. R. West, Solid State Chemistry and its Applications, John Wiley and Sons, New York, 1984.
3. A Carrington and A. D. Mclachlan, Introduction to Magnetic Resonance, Harper & Row, New York, 1979.
4. A Derome, Modern NMR Technique, Pergamon, 1983.
5. Farrar and E. D. Becker, Pulsed FT NMR Spectroscopy.
6. Wertz and Bolton, Electron Spin Resonance, McGraw Hill.

CHEM 544 MAGNETIC RESONANCE

Pre-requisites: CHEM 461, CHEM 541

SC; **Credits: 3**

UNIT – I

Magnetic Resonance - Description:

Classical and quantum description of magnetic resonance, Bloch's equations, complex susceptibilities, relaxation times, FID, FT techniques. Pulse experiments measurements of T1 and T2.

UNIT – II

Techniques in NMR:

FT-NMR spectroscopy, spin decoupling, NOE, 2D techniques – 2D J resolved spectroscopy, COSY.

NMR in solids: dipolar interactions second moments, Magic angle spinning.

UNIT – III

EPR – Review of Basic Concepts:

EPR of hydrogen atom, Free radicals in solution, spin densities, spin polarisation, anisotropy of Zeeman and hyperfine interaction. Spin labels.

UNIT – IV

EPR of transition Metal Ions:

s=1/2 systems, g and A anisotropy. Effect of spin orbit interaction. d^1 system in a tetragonal field. Covalency effects. Single crystal, powder and fluid epr spectra of transition ion (s = ½). S>1/2 systems, zero field splitting. EPR of metallo enzymes.

UNIT – V

Instrumentation in EPR & Spin-spin Interactions:

Basic EPR instrumentation. Advanced techniques: ENDOR, ELDOR, and ESEEM. Spin-spin coupled systems, Computer simulation techniques.

Recommended Books:

1. R.K. Harris: NMR spectroscopy
2. A. Carrington and A.D. McLachlon, Magnetic resonance, Harper & Row, 1967.
3. J. Pilbrow: Transition ion EPR (Oxford), 1968.

CHEM 546 ELECTROANALYTICAL TECHNIQUES

Pre-requisites: CHEM 442; **SC**; **Credits: 3**

UNIT – I

Kinetics of Electrode Reactions:

Mass transfer by Diffusion and Migration – models of electrode reactions – current potential characteristics – general mass transfer equation , migration and diffusion

UNIT – II

Potential Step Methods:

Types of techniques, step under diffusion control, Ilkovic equation – polarographic analysis – sampled current voltammetry: reversible, irreversible processes, multicomponent systems

UNIT – III

Chrono Methods:

Chronoamperometry, chronocoulometry – pulse polarographic methods: Tast pulse, normal pulse, differential pulse

UNIT – IV

Potential Sweep Methods:

Cyclic Voltammetry: Nernstian reversible, totally irreversible, quasi-reversible processes, multicomponent systems – convolute or semi-integral techniques

UNIT – V

Bulk Electrolysis Techniques: Classification of methods – Controlled Potential methods: current – time behaviour, electrogravimetry, electroseparation – Coulometric measurements: controlled current methods: characteristics, coulometric methods – Electrometric end point detection: classification, potentiometric, amperometric methods.

Recommended Books:

1. A. J. Bard and L. R. Faulkner, Electrochmical Methods, Fundamentals and applications, John Wiley, 1980
2. Bockris and Reddy, Electrochemistry, vol 1 & 2, Plenum, 1973.
3. H. Kissinger, Electroanalytical Techniques, John wiley, 1998
4. P. H. Reiger, Electrochemistry, Prientice Hall, 1987.

CHEM 562 COMPUTATIONAL QUANTUM CHEMISTRY

Prerequisites: CHEM 463 and CHEM 464;
SC*;* **Credits: 3**

UNIT – I

Programming and introduction to numerical methods:
Programming in Fortran and C languages. Least square Fit. Extrapolations and interpolations. Numerical differentiations and integrations.

UNIT – II

Self Consistent Theory of molecules: Roothan`s equations, Semi-empirical SCF methods. ab initio MO calculations. Basis sets. The Hartree-Fock limit. Correlation energy, Koopmans theorem. Perturbation theory and configuration interaction. Basis Set superposition error.

UNIT – III

Potential Energy & Surfaces:
Valence Bond configuration mixing diagrams. Rules for mixing VB configurations. VBCM and resonance theory. Reaction Profiles. Pontential energy surfaces. Curve crossing Model. Factors governing barrier heights.

UNIT – IV

Force field:
Quantum Mechanical and Molecular Mechanics potential functions. MM force fields. Parametrization. Steric energies, Heats of formation and strain.

UNIT – V

Computational Sessions:
Z-matrix specification, Input for Semi-empirical and *ab-initio* programs. Molecular mechanics program. Analysis of output.

Recommended Books:

1. J.P. Lowe: Quantum Chemistry, Academic Press, New York, 1978
2. U. Burkert and N.L. Allinger: Molecular Mechanics, ACS Monograph, 1977, American Chemical Society.
3. Albright, Burdett, and Whanghbo, Approximte Molecular Orbital Theory, Academic Press, 1985
4. MOPAC 6.0 Manual and computer program, QCPE edition.
5. PCMODEL Manual and Computer program, Serena Software

CHEM 580 PROJECT + *viva voce*

Pre-requisite: Consent of Teacher; **HC***;*
Credits: 5

Students are allotted to various faculties of the department according to their CPI and / or choice. They will be working on specialized problem related to the research interests of the respective guides.