M Sc Chemistry

2018 Syllabus

18CHY501 QUANTUM CHEMISTRY 3 0 0 3

Unit I: Quantum Chemistry - Introduction

Origin of quantum mechanics, de Broglie relationship, the uncertainty principle (no derivation); Postulates of quantum mechanics:postulate I – wave functions, postulate II- Operators in quantum mechanics, operator algebra, postulate-III – eigen values, eigen value equations, postulate IV – Expectation value, postulate V – time dependent and time independent Schrodinger equation

Unit II: Applying Schrodinger equation to various general systems

Translational motion of a quantum entity (particle in one dimensional box and three dimensional box); vibrational motion (harmonic oscillator); rotational motion (rigid rotator, particle on a ring and particle on a sphere); angular momentum.

Unit III: Atomic structure and chemical bonding

Hydrogen and hydrogen-like atoms; Multi electron systems- variation methods, perturbation methods,application to the ground state of Helium atom, SCF method, the exclusion principle

Chemical bonding: Hydrogen molecule ion and hydrogen molecule - molecular orbital and valence bond theory, homo and hetero nuclear diatomic molecules from VB and MO theory, the concept of directed valences and hybridization; quantum mechanics in band theory of metallic solids

Unit IV: Electronic structure of polyatomic systems: Computational quantum chemistry

Semi empirical and ab-initio methods; QM approximations, Details of HMO and EHMO and its application to chemical bonding in unsaturated molecules(ethylene, 1,3butadiene etc) ; Details of SCF procedure, Hartree and Hartree Fock methods (up to ground and excited states of hydrogen molecule); the basis sets, STOs and GTOs, nomenclature of basis sets, basis set errors, introductory ideas on DFT.

Unit V: Molecular properties: Computational quantum chemistry

Calculations of molecular properties like atomic charges, dipole moments, electronic distributions, vibration frequencies, NMR chemical shift etc using Gaussian program, specification of molecular geometry using Cartesian coordinates and internal coordinates, Z-matrix, Z-matrix of some simple molecules, structure of a Gaussian input file

TEXTBOOKS:


REFERENCES:


18CHY502 Concepts in Inorganic Chemistry 3 1 0 4

Unit 1 Nuclear Chemistry
Nuclear structure, mass and charge, mass defect, binding energy, stability rules, magic numbers, nuclear quantum numbers, nuclear parity and statistics, models of nucleus, shell model, liquid drop model, semi empirical mass equation, equations of radioactive decay and growth, half-life, average life determination of half-lives, nuclear reactions, energetics of nuclear reactions, types of nuclear reactions, spontaneous and induced fission, neutron capture cross sections - critical size principle and working of nuclear reactor. Numerical problems relevant to each session.

Unit 2 Radiation Chemistry
Radioactive elements, decay kinetics, parent-daughter decay relationships, radioactive equilibrium - transient and secular equilibrium, alpha and beta decay, gamma emission, Radiochemical methods - measurement of radioactivity, measurement of radiations - ionization chamber, proportional counter, the Geiger counter, scintillation counter, semiconductor detectors. Applications of nuclear and radiation chemistry, isotope dilution analysis - activation analysis, radioactive tracers, radiometric titrations, radiation dosimetry, hydrated electron.

Unit 3 Inorganic materials I
Alkali and alkaline earth metals, their compounds, crown ethers and cryptands as complexing agents for alkali metal ions, Be and Mg compounds, boron cage compounds, boron hydrides, structure and bonding, 3-centre-2-electron bonds, styx numbers, the importance of icosahedral frame work of boron atoms in boron chemistry, closo, nido and arachno structure, carboranes, metallocene carboranes, B-N compounds, interstitial compounds, metal carbides, nitrides and hydrides, fullerenes, functionalized fullerenes, C-nanotubes.

Unit 4 Inorganic materials II
Inorganic chains and polymers, rings, cages, and clusters, sulphur-nitrogen compounds, polymeric sulphur nitride, iso-poly anions, heteropoly anions, Keggin and Dawson polyoxometallates, borazines, metal clusters, nature of Si-Si bonds, silicates, silicates with zero-, one-, two- and three-dimensional structures, structure of elemental P, phosphonitrilic compounds, polymers with P-N bonds, interhalogen and pseudo halogens, intercalation chemistry, intercalation in layered materials like graphite, xenon fluorides & other xenon compounds.

Unit 5 Chemistry of f-block elements
The lanthanides and actinides, stable oxidation states, the lanthanide and actinide contractions, the f-orbitals, spectral and magnetic properties - comparison with inner transition and transition metals, separation of lanthanides, use of lanthanide compounds as shift reagents, photo-emission of lanthanide compounds, organometallic compounds of lanthanides and actinides and their structural features, reactions of lanthanide and actinide compounds, mineral sands of south west India - Ilmenite, Monazite, etc.

TEXTBOOKS:

REFERENCES:

**18CHY503 Principles in Organic Chemistry**

**Unit 1 Aromaticity**: Review of inductive and field effects – Resonance effects. Criteria for aromaticity – structural and electronic. Types – Hückel and Craig’s rule, homo (Five, Six, seven and eight, membered rings), hetero (furan, thiophene and pyrrole) and nonbenzenoid aromatic systems. Aromaticity of fused rings, annulenes, catenanes, rotaxanes, mesoionic compounds, metallocenes, cyclic carbocations and carbanions.

**Unit 2 Structure activity relationships**: Orientation effects of substituent, Quantitative treatment of structure on reactivity – free energy relationships – Hammet equations, Taft equation. Reactive Intermediates: Generation, structure and reactivity - reactions and rearrangement involving of carbocations - non-classical carbocations, carbanions, carbon radicals, radical ions, carbenes, nitrenes, isonitrenes, arynes.

**Unit 3 Mechanism and methods to determining them**: Thermodynamic and kinetic requirement, Baldwin rules for ring closure – Kinetic and thermodynamic control – Hammond postulates, microscopic reversibility, Marcus theory, methods of determining reaction mechanisms - solvents and their effect on course of a reaction.

Acids and Bases: Bronsted and Lewis acids - HSAB concept and bases, pH and pKa, effect of structure on acidity and basicity, effect of medium.

**Unit 4 Stereochemistry**: Optical and geometrical isomerism, absolute and relative configuration, Cahn-Ingold-Prelog system, prochirality, prochiral centre, atoms, groups and faces, designations. Atropisomerism, optical isomerism in biphenyls, allenes, spirans and “ansa” compounds, compounds containing chiral nitrogen and sulfur atom, geometrical isomerism of cyclic compounds, cumulenes and oximes. Asymmetric synthesis, stereoselective and stereospecific synthesis, regioselective and regiospecific reactions.

**Unit 5 Conformational Analysis**: Conformational analysis of cyclic and acyclic systems with special emphasis on six membered rings, conformational effects on the reactivity of acyclic and cyclic systems - elimination, substitution and addition, strain, structure and stability of small, medium, and large rings, anomic effect - cycloalkenes and cycloalkynes - kinetically and thermodynamically favoured products stereochemistry of SN1, SN2, SNi, E1 and E2 Selectivity in organic reactions: Chemoselectivity, regioselectivity, enantio- and stereo-selectivity. Stereosepects of the addition of X₂, HX, boranes and hydroxylation to C=C systems. *cis*- and *trans*- hydroxylation of cycloalkenes.

**TEXT BOOKS**

**REFERENCES**
Unit 1  Theories and Concepts on d-block Coordination Compounds

Introduction - ligands, nomenclature of coordination compounds, coordination compounds of d-block ions with coordination numbers of 2, 3, 4, 5, 6, 7 and 8. Werner’s coordination theory, Valence bond theory (VBT), Crystal field theory (CFT), CFSE, effects of CFSE on hydration energies and spinel groups (normal and inverse), types of ligands – spectrochemical series, spectral and magnetic properties (spin-only magnetic moments), nephelauxetic effect. Crystal field splitting patterns in complexes having Oh, Td, square planar, square pyramidal and trigonal pyramid geometries, factors affecting the magnitude of CFSE, various types of isomerism in coordination complexes, Jahn-Teller (JT) distortion, manifestation of JT on spectral properties. Molecular orbital theory (MOT), ligand field theory (LFT), molecular orbital energy level diagram for octahedral complexes without pi-bonding, metal-ligand pi-bonding, metal-metal multiple bonds, d-orbital based metal-metal σ, π and δ bonds in compounds like [Re₂Cl₈]²⁻, [Os₂Cl₈]²⁻, Cr₂(CH₃COO)₄ and R-Cr(I)-Cr(I)-R. Application of group theory to coordination compounds.

Unit 2  Reaction Mechanism

Complex equilibrium - formation constants, chelate and macrocyclic effects, factors affecting stability of complexes, methods of determination of stability constants, stability of complex ions in solutions, inert and labile complexes, mechanisms of ligand displacement and addition reactions in octahedral complexes and square planar complexes of platinum cis- and trans-effect, substitution reactions, mechanisms of substitution, kinetic consequences of reaction pathways, dissociation, interchange, association, dissociation, linear free energy relationships, conjugate base mechanism, stereochemistry of reactions (substitution in trans-complexes and substitution in cis-complexes), isomerisation of chelate rings, sigma-bonding and pi-bonding effects, oxidation-reduction reactions, inner and outer sphere electron transfer reactions, conditions for high and low oxidations numbers, reactions of coordinated ligands, hydrolysis of esters, amides and peptides, template reactions, electrophilic substitution, photochemical reactions of coordination compounds.

Unit 3  Coordination Chemistry of Inner-transition (f-block) Elements

f-block metal ions – oxidation states preferences, ligand preferences, coordination numbers and the geometry of the complexes, influence of lanthanide contraction and actinide contraction in their coordination behaviour, shapes of f-orbitals (4f and 5f), nature of bonding of f-orbitals with ligands, various types of coordination compounds of lanthanides and actinides, stereochemistry and reaction mechanism of f-block metal complexes.

Unit 4  Spectral Properties


Unit 5  Magnetic Properties

Magnetic properties of coordination complexes - magnetic susceptibility, contribution of spin-orbit coupling on μ_{eff} types of magnetic behavior - para-, ferro, anti-ferro and ferri-magnetic systems, Curie law, Curie-Wise law, Guoy, Faraday and superconducting quantum interference device (SQUID) methods, Kotani plots, giant magnetoresistance (GMR), anisotropic magnetoresistance (AMR) effect, effects of temperature on magnetic behavior, tunneling magnetoresistance (TMR). Magnetism of coordination complexes by multinuclear homo- and heterometallic 3d systems (also with exclusive 4d and 5d metal ions), mixed 3d-4f systems, importance of 4f-metal ions for functional applications. Nanoscale magnetic systems based on coordination complexes - Single Molecule Magnets (SMMs), Single Ion Magnets (SIMs), Single Chain Magnets (SCMs), Spin-crossover complexes, magnetic refringents (magnetic coolers), magnetic storage systems - magnetic random access memory (MRAM).
TEXTBOOKS:

REFERENCES:

18CHY505 GROUP THEORY AND ITS APPLICATIONS 3 0 0 3

Unit I Introduction to molecular point groups
Definition of a mathematical group, Symmetry in molecules, elements of symmetry, , matrix representation of symmetry operations, molecular point groups, , abelian group, cyclic group, symmetry operations as group elements, similarity transformation and classes, group multiplication table, symmetry classification of molecules into point groups (Schoenflies symbol)

Unit II Construction and interpretation of character tables
Reducible and irreducible representations, Great Orthogonality Theorem and its consequences, character tables, reduction formula, construction of character tables for point groups with order ≤6, interpretation of character tables.

Unit III Applications of Group theory - I (vibrational and electronic spectroscopy)
Infrared and Raman activity of molecular vibrations in H₂O, N₂F₂, BF₃, AB₄-type molecules (Td and D₄h) and AB₆ type (Oh) of molecules; selection rules; Electronic structure of free atoms and ions, splitting of terms in a chemical environment, construction of energy level diagrams, estimations of orbital energies, selection rules and polarizations, double groups, a brief idea on electronic spectra of transition metal complexes – selection rules, Orgel diagrams, Tanabe Sugano diagrams.

Unit IV: Applications of Group theory (Chemical bonding - Hybridization and molecular orbital formation)
Group theory to explain hybridization - wave functions as bases for irreducible representations, construction of hybrid orbitals for $AB_3$ (planar), $AB_4$ (Td), $AB_5$ ($D_{3h}$) and $AB_6$ ($O_h$) type of molecules, symmetry adapted linear combinations, projection operators, application of projection operators to pi-bonding in ethylene, cyclopropenyl systems and benzene, application of symmetry to predict polar and chiral compounds;

Unit V: Symmetry in solid state

Symmetry elements and operations in solid state – proper axis of rotation, mirror planes of symmetry, roto-reflection and roto-inversion axes of symmetry, screw axes of symmetry, glide planes; a brief introduction to the crystallographic point groups and space groups

TEXTBOOKS:

REFERENCES:
tion in a shared space, linear harmonic vibration, translational, rotational and vibrational partition function, molecular partition functions, partition functions and thermodynamic properties, calculation of equilibrium constant, heat capacity of gases, mono atomic solids, Einstein’s and Deby’s theory.

Unit 4 Equilibrium
Gibb’s free energy, direction of spontaneous change of a reaction, chemical potential, chemical potential and equilibrium, ΔG in terms of K, equilibrium constants – real gases and real reactions, equilibrium respond to catalyst, temperature, pressure and pH, application of ΔG and K – extraction of metals from their oxides, Ellingham diagram, and thermodynamics of ATP & respiration, biological energy conversion.

Unit 5 Phase Equilibrium
Gibb’s Phase rule, one component system, two component systems, vapour pressure diagrams and their interpretation, lever rule, temperature-composition diagrams, liquid-liquid phase diagrams, distillation of partially miscible liquids, azeotropes, liquid-solid phase diagrams, phase diagram for the system Na/K/Na2K, phase diagram - steel, alloys, Fe-C system, zone refining, three component system, triangular coordinates, three component system – partially miscible liquids - H2O/CHCl3/CH3COOH, phase diagram - NH4Cl/(NH4)2SO4/H2O

TEXTBOOKS:

REFERENCES:

18CHY512 MOLECULAR SPECTROSCOPY 3 1 0 4

Unit 1 Rotational and Vibrational Spectroscopy
Introduction to spectroscopy, rotation spectra - diatomic and polyatomic molecules, selection rules, intensities of spectral lines, stark effect, instrumentation of micro wave spectroscopy, applications and structural determinations, vibration spectra of diatomic molecules, harmonic and anharmonic vibrations, diatomic vibrating rotor, selection rule, breakdown of Born Oppenheimer approximation, rotational character of vibration spectra, different modes of vibrations, vibration-rotation spectra, Fermi resonance, vibration spectra of polyatomic molecules, IR spectra of organic and inorganic compounds, phase, temperature and solvent dependence, FTIR technique, instrumentation, Raman spectra (including the use of laser) - theory, relation with IR spectroscopy, mutual exclusion principle, resonance Raman, stimulated hyper and inverse Raman effects, instrumentation and applications of Raman spectroscopy.
Unit 2 UV-Visible and Fluorescence Spectroscopy

Electronic spectra of atoms - single and multi electron systems, j-j and L-S coupling, electronic spectra of diatomic and polyatomic molecules, its relation to electronic arrangement and symmetry of molecules, application of group theory in electronic spectra, selection rules, nature of electronic excitation, principles of absorption spectroscopy, Beer-Lambert law, presentation of spectra, chromophores, forbidden transition, different types of electronic transitions, p-p*, n-p* etc transitions, nature of transitions in carbonyl compounds, the effect of conjugation, effect of conjugation on alkenes, HOMOs and LUMOs, Woodward-Fieser rules for dienes, spectra of carbonyl compounds, enones, Woodward rule for enones, spectra of aromatic compounds, effect of substituents, structural information from electronic spectra, excited states of molecules, fluorescence and phosphorescence, Jablonski diagram in detail, lifetime of excited states, quantum yields, photosensitization, application of UV-Visible and Fluorescence Spectroscopy for structural elucidation of organic compounds, diffuse reflectance spectra.

Unit 3 NMR Spectroscopy

Nuclear magnetic resonance phenomenon - theory, relaxation effects, NMR uses active nuclei, Fourier Transformation in NMR, measurement of relaxation time, chemical shift, magnetic anisotropic effect, multiplets in NMR, spin-spin splitting, n + 1 rule, Pascal’s triangle, tree-diagram, spin-spin splitting constant, J, 2J and 3J and long-range coupling, measurement of J, Karplus relationship, first and second order spectra, AX, AB, AX2, AX3, A2X3, AMX type spectra, double resonance and spin tickling, chemical shift reagents, spectra in higher fields, spectra of conformational isomers, homotopic, enantiotropic and diastereotopic systems, C13 spectra, factors related to 13C spectra, 1H coupled 13C spectra, 1H decoupled 13C spectra, chemical shift values, nuclear Overhauser effect (NOE), cross-polarization, off-resonance resonance decoupling, application of 1H and 13C NMR spectroscopy for the structural elucidation of organic compounds, 11B, 15N, 19F and 31P NMR spectra, spectra of paramagnetic complexes, magnetic susceptibility, contact shift, fluxional molecules and their studies using NMR, solid state NMR.

Unit 4 ESR, NQR and Mossbauer Spectroscopy

ESR spectroscopy - theory, hyperfine and superfine splitting, ESR active simple organic systems, ESR of inorganic systems like Cu2+ and VO2+ complexes, ‘g’ markers like DPPH and TCNE, evaluation of spin Hamiltonian like A, gll, g-, covalency factor in Cu2+ complexes, analysis of ESR spectra of VO2+ complexes, NQR spectroscopy - theory, relationship between electric field gradient and molecular structure, quadrupole coupling constant and structural information of compounds, Mossbauer spectroscopy, principle, Doppler effect, isomer shift, Zeeman splitting, quadrupole splitting, application of Mossbauer spectroscopy for studying Fe and Sn compounds and phase transformation, application of ESR spectroscopy.

Unit 5 Mass Spectrometry and PES

Mass spectroscopy, base peak and molecular ion peak, isotope ratio data, fragmentation patterns of alkanes, alkenes, alkynes, aromatic hydrocarbons, alcohols, phenols, aldehydes, ketones, esters, carboxylic acids, amines, methods of desorption and ionization (EI, CI, LD, MALDI, PD, FAB, SIMS), MS/MS and determination of molecular formula, metastable ions and their significance, study of fragmentation pattern, application of MS in structural elucidation and other frontiers of science, application of MS for quantitative analysis, photoelectron spectroscopy (PES), principle, application of PES. Structure determination using IR, UV-visible, NMR, MS and ESR spectral techniques.

TEXTBOOKS:
Unit 1 Nucleophilic Substitution: SN1, SN2, and Borderline (ion pair), SNi, SET mechanisms, Neighbor- 
group participation, substitution at allylic carbons, substitution at aliphatic trigonal carbon, substitution at vin-
nylic carbon. Effect of substrate structure, nucleophile, leaving group and medium on reactivity. Ambident 
nucleophiles and substrates. Aromatic nucleophilic substitution: SNAr, SN1, benzene and SRN1 mechan-
isms. Effect of substrate structure, leaving group and attacking nucleophile on reactivity.

Unit 2 Electrophilic substitution: SE2 and SEi, SE1, substitution accompanied by double bond shift. Effect of 
substrate, leaving group, and solvent on reactivity. Aromatic electrophilic substitution: Arenium mechanism,
Structure – reactivity relationship, substituent effect, o/p ratio, ipso substitution, orientation and reactivity,
quantitative treatment.

Free radical reactions: Radical addition. Effect of substrate (aliphatic, aromatic, bridgehead), nature of the 
radical and solvent on reactivity.

Unit 3 Addition reactions: Mechanism of Electrophilic, nucleophilic and radical addition. Addition to conju-
gated systems. Orientation and reactivity. Addition of hydrogen halides, Oxymercuration, halogenation, sul-
fenylation, selenylation, addition involving epoxides, addition via organoborane. Addition of water, alcohol,
sulfides, to aldehydes, ketones, imines, isothiocyanates, nitrocompounds, nitriles. Mannich reaction,
Elimination reactions: Mechanism of elimination reactions E2, E1, E1CB, steric effect. Effect of substrate 
structure, base, leaving group and medium on reactivity. Mechanism of pyrolytic elimination.

Unit 4 Rearrangement reaction: Mechanism of Nucleophilic, electrophilic and radical rearrangements. Na-
ture of migration, migratory aptitudes, memory effects. Wagner-Meerwein, Pinacol, Demyanov, diene-
phenol, Benzil-Benzilic acid, Favorskii, Wolff, Neber, Hofmann, Curtius, Lossen, Schmidt, Beckmann,
Baeyer-Villiger, Stevens, benzidine, Hofmann-Loffler and Chapman rearrangements and their mechanisms.

Unit 5 Photochemistry and pericyclic reactions: General principles – Fate of excited state – Jablonsky dia-
gen - chemical process – Photochemistry of alkenes, dienes and polyenes, Carbonyl compounds, Norrish 
type 1 and Type 2, Patterno –Buchi reaction.

Pericyclic reactions: Cyclo addition - Diels-Alder reaction, Substituent effect on reactivity, regioselectivity 
and stereochemistry, Catalysis of Lewis acids, Synthetic applications, Enantio selective Diels alder reactions,

TEXT BOOKS

REFERENCES

18CHY514 Heterocyclic and Natural Product chemistry 3 0 0 3

Unit 1 Heterocyclic compounds
Nomenclature and general characteristics of heterocyclic compounds, study of three and four-membered ring heterocycles containing one heteroatom, structure and synthesis of penicillin and cephalosporin-C, structure and synthesis of reserpine, heteroaromatic compounds (five and six-membered rings) containing one and two heteroatoms, fused ring compounds - indole, quinoline, isoquinoline, coumarin, flavones, purine and pyrimidine, bases present in nucleosides.

Unit 2 Carbohydrates and nucleic acids

Unit 3 Chemistry of Natural Products
Alkaloids - classification, structure elucidation based on degradative reactions (quinine atropine), Terpenoids - classification, structure elucidation and synthesis of abietic acid, terpenoids. Total synthesis of quinine and papaverine (morphine, heroin).

Unit 4 Steroids
Steroids - classification, structure of cholesterol, conversion of cholesterol to progesterone, androsterone and testosterone, classification, structure and synthesis of prostaglandins, biosynthesis of fatty acids, prostaglandins, and steroids.

Unit 5 Amino acids, Peptides and Enzymes
Synthesis of amino acids - Strecker and azlactone synthesis, reactions of amino acids, structure of proteins, introduction to enzymes and coenzymes with special reference to the function of chymotrypsin, NAD, thiamine, pyridoxal, solid phase synthesis – choice of resin, classification and reactions leading to peptide formation.
TEXT BOOKS
2. Sujata V. Bhat, Bhimsen A. Nagasampagi, Meenakshi Sivakumar, Chemistry of Natural Products, Springer 2005

REFERENCES
2. Ashutosh kar, Chemistry of Natural Products, (Volume I and II), CBS

18CHY515  Organometallic Chemistry  3 0 0 3

Unit 1: Concepts and Metal Carbons
History and overview on organometallic compounds. Classification and nomenclature – hapticity of fragments, 18-electron and 16-electron organometallic compounds. Structure prediction based on ’18 electron rule’. Metal carbons – synthesis and bonding of metal carbons (based on MO theory), donor and acceptor properties of CO, different types of binding modes of CO, polynuclear carbons with and without bridging groups, metal-metal bonding in M-CO clusters, cluster valence electron (CVE) count, CVE based structure prediction. IR spectral features of metal carbons, activation of CO by bonding with metal ions.

Unit 2: Types of organometallic compounds
Metal phosphines compounds of transition metals, M-N₂ (metal dioxygen), M-O₂ (metal dioxygen), M-NO (metal nitroso) and M-CN (metal cyanide/isocyanide) complexes, bonding and structural features. Organometallic compounds with π-donor ligands like olefins, acetylenes and allyl moieties. Metal derivatives of cyclic π-donors (metallicenes, sandwich/half-sandwich compounds, bent metalloccenes), metal-carbon σ-donors (metal carbenes – Fischer carbenes, Schrock carbenes and N-heterocyclic carbenes, metal polyenes, metal carbanes, metal alkyl/aryl derivatives). Organometallic chemistry of lithium and magnesium, aluminum alkyls and all other main-group organometallics. Structural features and nature of bonding in above compounds.

Unit 3: Structure and Bonding
Fragment molecular orbitals (FMO) of various organic and inorganic moieties like CH₃, CH₂, CH, BH₂, BH, NH₂, NH. FMO’s (π-orbitals) of C₃H₅, C₄H₄, C₅H₅, C₆H₆, C₇H₇. Inorganic fragments MLₙ with varying number of L’s. Symmetry and shape of their FMO’s. Isolobal concept, iso-electronic and isolobal relationships between various organic and inorganic (MLₙ) fragments. Structure and bonding between various organic and inorganic fragments based on MO level diagrams – metal-olefins, MLₙ-cyclobutadiene, MLₙ-carbene, MLₙ-carbyne, MLₙ-cyclopentadienyl systems, compounds with metal-metal multiple bonds (metal-metal σ, π and δ bonds).

Unit 4: Stereochemistry and reactions
Stereochemically non-rigid molecules, fluxional nature of organometallic compounds (including Li-C, Mg-C), characterization of non-rigidity of organometallic compounds by NMR spectroscopy. Difference in NMR spectra of fluxional organometallic compounds at high and low temperatures. Characterization techniques of organometallic compounds (by NMR – ¹H, ¹³C and ³¹P NMR spectroscopy, Dynamic NMR, Mass spectrometry). Reactions involving various organometallic compounds - oxidative addition reactions, reductive elimination reactions, migratory insertion reactions, 1,1-type and 1,2-type insertion reactions, elimination reactions, β-hydride elimination reactions. Conditions for organometallic compounds to exhibit above reactions, cyclo-metalation and ortho-metalation reactions, agostic interactions.

Unit 5: Organometallic Catalysis
Alkene hydrogenation using Wilkinson’s catalyst, water-gas shift reaction, Mosanto process, Cativa Process. Reaction steps in the above catalytic processes. Hydro-formylation reactions, catalytic addition of molecular oxygen to alkenes (Wacker process), Ziegler-Natta polymerization of alkenes, Fischer-Tropsch process, ole-
fin-metathesis (types of Grubbs catalysts and Hoveyda–Grubbs catalysts), oligomerization of alkynes, aluminum alkyls in polymerization of olefins. Palladium based reactions such as Heck, Stille, Suzuki, Sonogashira, Buchwald-Hartwig couplings; Tsuji-Trost C-C bond formations. Homogeneous vs. heterogeneous organometallic catalysis (principles, mechanism and their applications). Organometallics - in industry, in medicine, in agriculture and in environmental science.

TEXTBOOKS:
5. J.D. Atwood, ‘Inorganic and Organometallic Reaction Mechanism’, 2nd Edn., Wiley-
REFERENCES:

18CHY581 INORGANIC SEMI-MICRO QUALITATIVE ANALYSIS LAB. 0 0 6 2

Semi micro analysis of mixtures
The mixture will include 4 cations including two common (eg. Cations of metals like Cu, Mn, Zn, Ni, Ca, Ba, Mg etc) and two less common cations (eg. Cations of metals like Ti, Zr, V, W, Li, Ce, Th etc).

(The student has to successfully analyze a minimum of 10 mixtures).

TEXTBOOKS:

REFERENCES:
A. Estimations:
Estimation of equivalent weight of an acid
Estimation of glucose
Estimation of phenol
Estimation of acetone
Estimation of acid value of an oil
Estimation of iodine value and sap value of an oil
Estimation of Nitrogen – Kjeldahl method
Estimation of formaldehyde
Estimation of aniline
Estimation of ester

B. Preparations of Organic Compounds
Double stage preparations
(a) m-nitro benzoic acid from ethyl benzoate
(b) p-bromobenzanilide from aniline
(c) p-nitro acetanilide from aniline

Single stage preparations
(a) Benzimidazole
(b) Benzophenone oxime
(c) Dibenzilidene acetone (chalcone)
(d) Benzalacetophenone
(e) Benzanilide
(f) Acetanilide
(g) Acetyl salicylic acid (aspirin)

Name Reactions
(a) Benzil-Benzilic acid rearrangement
(b) Cannizaro reaction
(c) Claisen condensation

For all preparations
1. TLC to be done and Rf values of each compound to be reported
2. Melting point of pure compounds to be found
3. A small portion should be recrystallised from suitable solvent
4. Purified products to be displayed
5. Mechanisms for each preparation should be suggested

REFERENCES:
1. Construction of phase diagram for three component system.
2. Determination of equivalent conductance at infinite dilution of weak electrolytes.
3. Determination of order of reaction for ion exchange reaction.
4. Extraction efficiency of solute from a solution by immiscible solvent method.
5. Determination of calorific value using Bomb calorimeter.
7. Determination of the formation constant of silver-ammonia complex and stoichiometry of the complex potentiometrically.
8. Determination of flash point, fire point of a lubricant.
9. Determination of cloud point and pour point of a lubricant.

TEXTBOOKS:

REFERENCE BOOKS:

18CHY584 INORGANIC QUANTITATIVE ANALYSIS LAB. 0 0 6 2

1. Estimation of Calcium (Permanganometry)
2. Estimation of Barium (Iodometry)
3. Estimation of Calcium as Calcium Carbonate (Gravimetry)
4. Estimation of Zinc using oxine (Gravimetry)
5. Estimation of Iron as Ferric Oxide (Gravimetry)
6. Analysis of Brass
7. Estimation of Copper and Nickel in a Mixture
8. Estimation of Copper and Iron in a Mixture
9. Preparation and Determination of Ferrous Oxalate
10. Estimation of Different Types of Hardness in the Given Water Sample
11. Estimation of Different Types of Alkalinitities in the Given Water Sample
12. Estimation of Dissolved Oxygen in the Given Water Sample
13. Complexometric Estimations

TEXTBOOKS:

REFERENCES
18CHY601 ELECTROCHEMISTRY KINETICS AND SURFACE CHEMISTRY 3104

Unit 1 Surface Chemistry
Different types of interfaces, molecular and atomic surface structure, surface chemical reactions, surface tension of solutions, surface excess, thermodynamics of surfaces, Gibbs equation and its derivation, surface films, surface potential.
Adsorption by solids, Langmuir isotherm - its kinetic and statistical derivation, Freundlich equation, multilayer adsorption, BET isotherm -its kinetic derivation, measurement of surface area.
Colloids - their preparation, purification, stability & electro kinetic phenomena, Donnan membrane equilibrium, micro and nano emulsions.
Surface analysis using photoelectron spectroscopy, surface imaging techniques like SEM, TEM, AFM etc., sputter coating, ion beam principles, design of surfaces with novel properties.

Unit 2 Electrochemistry I

Unit 3 Electrochemistry II
Electrochemical cells, standard electrode potentials, reversible cell, concentration cells with and without Electrochemical cells, standard electrode potentials, reversible cell, cell notation and calculation of emf – variation of potential with concentration, pressure and temperature – concentration cells with and without transference, Liquid Junction Potential – its calculation and elimination - Thermodynamics of cell reactions and equilibrium constant - applications of e.m.f. measurements, potentiometric measurement of pH – reference electrodes - glass and quin-hydrone electrodes and their performance and limitations, - ion selective electrodes – biomembranes, Interfacial region – electrical double layers and their structure – Helmholtz-Perrin, Gouy-Chapman and Stern models - charge transfer across interfaces, mass transport – diffusion and convection controlled transport – irreversible electrode processes - activation, concentration and IR polarisation, decomposition potential, Butler-Vohmer equation - over potential (hydrogen, oxygen and metal decomposition over voltage), theories of over voltage, Tafel equation, and Tafel plots – corrosion and its rate from Tafel equation.

Unit 4 Chemical Kinetics I
Reaction rates and order of reactions, determination of order of reactions, complex reactions, reversible, consecutive and concurrent reactions, reactions of variable order, steady state treatment, reaction mechanism and molecularity, theories of unimolecular reactions and termolecular reactions, Arrhenius equation, collision theory and transition state theory, comparative study of the theories of reaction rates, free energy of activation, effect of solvent on rate of reactions, ionic reactions and effect of ionic strength - salt effect, effect of pressure on velocity of gas reactions.

Unit 5 Chemical Kinetics II
Reaction dynamics, fast reactions, flash photolysis and relaxation methods, catalysis and inhibition, homogeneous catalysis, acid, base and enzyme catalysis, kinetics of enzyme catalyzed reaction - the Michaelis-

**TEXTBOOKS:**

**REFERENCES:**

**18CHY602 Synthetic Strategies and Reagents 3104**

**Unit 1 Synthetic Strategies**

**Unit 2 Oxidation and reduction:**
PCC, DDQ, DMSO, Dess-Martin Reagent, TEMPO, osmium tetroxide, ruthenium tetroxide, selenium dioxide, peracids, hydrogen peroxide, singlet oxygen, aluminium isopropoxide, periodic acid, lead tetraacetate. Swern, Jones, Oppeneur oxidation, Woodward and Prevost hydroxylation, Sharpless asymmetric epoxidation, catalytic hydrogenations (heterogeneous and homogeneous), Clemmenson, Wolff Kishner, Rosenmund and MPV reductions, metal hydrides as reagents (aluminium/boron hydrides and hydroboration reaction), Birch reduction, Borsche Reduction, hydrazine and diimide reduction.

**Unit 3 Organometallic reagents:** Preparation, properties and reactions of organo lithium, organosilicon, organozinc (Reformatsky reaction) and organomagnesium reagents (Barbier and Grignard), organocadmium, organo mercury reagents based organometallic reactions involving C-C bond formation. Selected functional group transformations in organic synthesis. Preparation and reactions of Organo copper, organopalladium,- Wacker process – Heck reaction, cross coupling, carbylonylation reaction, organonickel, organo cobalt and organo rhodium reagents – Olefin metathesis reaction. Reactions and applications of Organoboron, organo silicon and organotin compounds.

**Unit 4 C-C, bond formation**

**Unit 5C-N, C-O bond formations**
C-O bond formation – Barton, Fischer esterification, Prins, Darzen, Baeyer-Villiger, Mitsunobu, Williamson’s ether synthesis, Ullman Coupling with Boronic Acids.

**TEXT BOOKS**

REFERENCES

18CHY603 Solid State Chemistry and Materials Science 3 0 0 3

Unit 1 Introduction to Crystal Systems
Introduction to solids - solid state chemistry, close packing, hcp, fcc, density, coordination numbers, tetrahedral and octahedral holes, body centered and primitive structures, symmetry, proper rotation, mirror planes, inversion, improper axis symmetry elements, symmetry in crystals, Schoenflies and Hermann-Mauguin notations, unit cells, glide plane, screw axis, atom occupancy in cubic unit cells, seven crystal systems/classes, space groups, Miller indices, Bravais lattices, reciprocal lattice, inter-planar spacing in different crystal systems, fractional coordinates, ionic solids, structures of CsCl, NaCl, NiAs, zinc blende and wurtzite structures, MX2 type solids, fluorite and antfluorite structures, CdCl2 and Cd2 structures, rutile and anti-rutile, ReO3, spinel and inverse spinel, pervoskite structures, ionic radii, crystal radii, radius ratio, Extended covalent array, diamond, graphite.

Unit 2 Bonding in Solids and Electronic properties
Bonding in crystals, metallic bonding, ionic bonding, covalent bonding, silicates, Born-Haber cycle, Hess’s law, lattice energy (L) and calculation of L, free electron theory, density of states, electronic conductivity, molecular orbital theory, overlap and bonding, linear chain of H atoms, LCAO, Fermi Level, conductors, insulators and semiconductors, n- and p-type semiconductors, bands in compounds, band-gap energy, direct and indirect band gaps in semiconductors, band-gap measurements, electrical conductivity, photoconductivity.

Unit 3 Magnetic and Optical Properties of Solids

Unit 4 Materials Science-Structure and properties
Solid materials of importance. Structure and properties of SiO2, ZrO2, SiC, BN, ZnO, TiO2, CdS, CdTe, GaAs, MoS2. Band-gap properties of semiconductors like ZnO, TiO2, CdS, CdSe, CdTe, GaAs, MoS2 and (CH3NH3)PbX3-type perovskites. Photo-catalytic properties of ZnO and TiO2 – principle and applications. Inorganic-organic hybrid materials. High Tc superconductors (HTS) like Bi-Sr-Ca-Cu oxide based HTS (BSCCO) and Y-Ba-Cu-oxide (YBCO), their structure and properties. Metal-organic framework (MOF) materials, special features of MOF materials. Synthesis, special features and properties of MOF materials like...
HKUST-1 and MOF-8. Gas storage and emission properties of MOF materials. MOFs as sensors. Zeolites, their special features and properties.

**Unit 5  Materials Science-Synthesis, processing and characterization**


**TEXTBOOKS:**
1. L V Azroff, 'Introduction to Solids', Tata McGraw-Hill publishing company

**REFERENCES**
5. F.H. Norton, Elements of Ceramics,

**18CHY604  Bio-inorganic Chemistry  3 0 0 3**

**Unit 1: Basics in bio-inorganic chemistry**

Essential elements in biological systems, transport of ions across biological membranes, active and passive transport, metal transport and metallochaperons, Na⁺/K⁺ pump and active transport. Metal complexation with biological molecules. Electron transport in biology, electron transport chain (ETC), role of ETC in biological systems. Amino acids, peptides and proteins, primary and secondary structure of proteins, α-helix and β-sheets forms of proteins and their special features; tertiary and quaternary structures of proteins the type of molecular interactions involved in them . Reactive oxygen species (ROS), generation and function of organic free radicals, action of ROS in biological systems, oxidative stress, antioxidants. Photosynthesis, PS-I and PS-II.

**Unit 2: Oxygen take-up, transport and storage proteins**

Porphine, corrin, corrole, chlorin and bacteriochlorin. Myoglobin (Mb) and hemoglobin (Hb), their prosthetic groups and functions, mechanism for reversible binding of O₂ in Mb and Hb. Cooperative effect in Hb and its consequence. Behaviour of bound O₂ to Fe(II). Difference between O₂ and CO binding to Hb and Mb, CN⁻ poisoning. Structure and functions of haemerythrin (Hr) and haemocyanin (Hc), O₂ binding nature in Hr and Hc, electron transfer processes in them. Cytochromes and their role in biology, cytochrome P-450, cyto-
chrome C-oxidase and oxygen transfer from O₂ to non-activated substrates, monooxygenases, methane monooxygenase (MMO). Fe-S and other non-heme iron proteins, ferredoxins-their structure and special properties, transferrin, ferritin, siderophores, enterobactin, uptake, transport and storage of iron. Sickle-cell anemia

Unit 3: Metallo-enzymes

Unit 4: Other functional roles of metal ions
Zn in biological systems, Zn-finger proteins – structural features and properties, classifications and their roles in biological systems. Ca²⁺ binding proteins, calmodulins. Metal ion based (Pt, V, Au) drugs, anticancer agents. Cis-platin and its properties. Chelation therapy, macrocyclic antibiotics. Role of Mn, Ni, Mo and Cr in biological systems, metal toxicity and homeostasis, therapeutic complexes. Diseases caused by both excess and deficiency of metal ions, thalassaemia, Wilson disease. DNA intercalators, diagnostic agents, MRI imaging and contrast agents, the role of Gd³⁺ and other metal ions as contrast agents.

Unit 5: Biomimetic compounds, metals in medicine
Porphyrins (H₂P) and metalloporphyrins (MP), spectral, fluorescence and redox properties of H₂P and MP. Biomimetic compounds. Fe(II), Co(II) and Cu(II) based model compounds model compounds of Mb and Hc –, ‘picket-fence’ porphyrin and its special features. Photodynamic therapy (PDT), principles and applications. Natural and synthetic ionophores, crown ethers, interaction and uptake of alkali metal and alkaline earth metal ions with crown ethers, cryptands and cryptates, calixarenes and their special properties, cyclo-dextrins and their special properties.

TEXTBOOKS:

REFERENCES
Unit 2: Industrial Cathodic process - Electrodeposition of copper, nickel and chromium over mild steel – zinc plat ing on MS – decorative plating of silver and gold – nano plating and microstructure of deposits - Tests for adhesion, hardness, thickness, uniformity and corrosion resistance of the electro deposits-post plating passivation processes-barrel plating of small components - Electroless deposition of nickel, copper, gold on metal components – making of wave-guides and plated through hole boards -

Unit 3: Industrial Anodic Processes: Anodising of aluminium and its alloys – baths used, operating conditions and se-QUENCE determination of thickness – industrial applications- nano anodizing of titanium, and tantalum – application to sensor field

Electropolishing of ferrous and non-ferrous metals and alloys - mechanism of electropolishing –Electrochemical etching of ferrous and non-ferrous metals –

Special processes: Electrolysis of water – electrowinning of aluminium and sodium – electrolysis of brine-phoetochemistry

Unit4 - Electrochemical energy systems: Primary batteries: Zinc-carbon (Leclanche type), zinc alkaline (Duracell); li-thium primary cells - liquid cathode, solid cathode and lithium-ferrous sulphide cells Secondary batteries: Lead acid and VRLA (valve regulated (sealed) lead acid), nickel-cadmium, nickel-zinc, nickel-metal hydride batteries, lithium ion batteries, ultra thin lithium polymer cells (comparative account) Advanced Batteries for electric vehicles, requirements of the battery - sodium-beta and redox batteries. Reserve batteries thermally activated batteries - remote activation - pyrotechnic materials: Fuel Cells: Principle, proton exchange membrane (PEM), direct methanol(DMFC), molten carbonate electrolyte (MCFC) fuel cells and outline of biochemical fuel cells.

Unit5 - Electro chemical sensors: Potentiometric sensors, solid state Potentiometric chemical sensors, polymeric membrane sensors, ion selective field effect transistor, application, Hydrovolumetric technique-hydrodynamic vol-tammetric-application, voltammetric sensors-electrode modification application, optical sensors,-bioamperometric titration. Methods involving forced convection-hydrodynamic methods

Text books

References
**Unit 2** Quantification of Enzymes and their substrates

**Unit 3** Immobilized enzymes
Immobilization methods - nanoparticleing covalent immobilization, Crosslinking with bifunctional reagents. Properties of immobilized enzymes, immobilized enzyme reactions, theoretical treatment of packed bed enzyme reactors.

**Unit 4** Antibodies
Structural and functional properties of antibodies, Polyclonal and monoclonal antibodies Antibody-antigen interactions, analytical application of secondary antibody-antigen.

**Unit 5** Biosensors

**TEXTBOOKS:**

**REFERENCE:**

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**18CHY633 CHEMISTRY OF BIOMOLECULES 3003**

**Unit 1 Amino acids, Proteins and Peptides**
Classification, Stereochemical aspects, physical properties, Ionic properties, spectral properties, essential and non essential amino acids, chemical reactions of amino acids, Industrial preparation and chemical synthesis of amino acids. Ionic properties of proteins, protein structure, protein purification, protein structure determination, proteomics and protein function, solid phase peptide synthesis, biologically important peptides.

**Unit 2 Enzymes**
Introduction to Enzymes, Classification of enzymes, mechanism of enzyme action, immobilized enzymes and enzyme technology, enzyme analog built polymers, design of molecular clefts, enzymes in synthetic organic chemistry. Enzymes in biological systems.

**Unit 3 Molecular biology and bioinformatics**
Structure of nucleic acids, genes and genome complexity, functions of nucleic acids, isolation and separation of nucleic acids, molecular analysis of nucleic acid sequences, nucleotide sequencing of DNA.

**Unit 4 Immunochemical techniques**
Production of antibodies, purification and fragmentation of immunoglobulins, immunoprecipitation, labeling antibodies, immunoblotting, immunoassays, immunohisto/cytochemistry.
Unit 5 Recombinant DNA and genetic analysis
Constructing gene libraries, cloning vectors, hybridization and gene probes, application of gene cloning, expression of foreign genes, pharmacogenomics.

REFERENCES:

18CHY634 INDUSTRIAL CHEMISTRY 3003

Unit 1 Water treatment
Softening of water, Ion exchange process, Lime soda process, Modified Lime soda process, Zeolite process, Chemical and physical method of sterilization, Desalination, Boiler problems. Corrosion of boiler units, industrial water treatment, water analysis.

Unit 2 Fuels
Calorific value, determination of Calorific value, classification of fuels, Solid fuels, Properties of fuels, classification of coal, coking and non-coking coals, advantages and disadvantages of solid fuels. Liquid fuels, gaseous fuels, analysis of fuel gases, Distillation of petroleum. Processing & purification of petroleum and petroleum products, Flash point, Fire point, Knocking, antiknocking, Cetane number, octane number, natural gasoline, cracking, polymerization, alkylation, isomerisation, rocket fules, fossil fules, nuclear fuels.

Unit 3 Energy resources
Renewable and non renewable sources of energy, conventional and non conventional sources of energy, solar energy, solar technology, solar photovoltaic cell - application, PV lantern system, Radiotelephone system, Application of solar energy, Environmental implication, Nuclear energy, nuclear fuel cycle in India, Energy conservation and waste heat boilers, Fuel cells, hydrogen cells.

Unit 4 Paints and Pigments
White pigment, blue, green, yellow, black and red pigments - manufacture, physical properties, characteristics, Manufacture of paints, setting of paints, requirement for good paints, emulsion paint, latex paint, luminescent paint, fire retardant paints, heat resistant paints, varnishes, manufacture of varnishes, enamels, lacquers.

Unit 5 Explosives and Toxic Chemical Weapons
Introduction, Classification. Deflagrating or low explosives. Characteristics of explosives, nitrocellulose, PETN, DNB, TNB, TNT, Picric Acid, Nitroglycerine, Dynamite, Cirdite, Gun powder, RDX, EDNA, HMX,Tetryl, Pentryl, Hexyl, Dinol. Toxic chemical weapons, screening smokes, Incendiaries, Pyrotechniques, Explosives in India.

TEXTBOOKS:

REFERENCES

18CHY635 INDUSTRIAL STOICHIOMETRY 3 0 0 3

Unit 1 Introduction to process calculation - dimensions and systems of units - fundamental quantities of units, derived quantities, definition and units of force, volume, pressure, work, energy, power, heat-unit conversions in FPS, MKS and SI systems.


Unit 3 Description and simple material balance calculation of physical processes such as drying, distillation, absorption, mixing, crystallization, Evaporation.

Unit 4 Single stage material balance calculation of leaching and extraction, calculations involving recycling and by passing operation - limiting reactant, excess reactant, conversion, yield and selectivity - simple numerical for finding yield, conversion and composition.

Unit 5 Calculation of material and energy balance based on reactions involving heat capacity and specific heat - mean heat capacity of gases - heat capacity of gas mixture and liquid mixture. Calculations of heat capacity by integral equation up to three terms - sensible and latent heats of fusion, sublimation, vaporization. Calculations of standard heat of formation from heat of combustion data. Calculations for heat of reaction from heat of formation and heat of combustion data – Fuels - calorific values proximate and ultimate analysis - air requirement and composition of flue gases.

TEXTBOOKS:

REFERENCE BOOKS:

18CHY636 MATERIAL SCIENCE AND NANOCHEMISTRY 3 0 0 3

Unit 1 Introduction to Nanomaterials Introduction to Material Science, Interdisciplinary nature, Structure of nanomaterials, Length scales, de-Broglie wavelength & exciton Bohr radius, Foundations of Quantum Mechanics: wave function, Schrödinger equation, uncertainty principle, quantum wells, quantum wires, quantum dots, articles.

Unit 2 Nanomaterials: Synthesis, Properties Size effect and properties of Nanoparticles - Particle size - Particle shape - Particle density, Specific surface area and pore - Composite structure, Crystal structure - Functionality of nanostructures and their characteristic evaluation - Optical properties - Catalytic property; Synthesis - Methods and Strategies, Top-down and bottom-up approaches, Chemical vapor deposition, Laser ablation, Electric-arc, Sol-Gel Processing, Lithography - Surface modification of inorganic nanoparticles by organic functional groups.

Unit 3 Surface Science and Characterization of Nanomaterials Electron Microscopy, MFM, SNOM, SEM, TEM, EDAX, X-ray Diffraction and Electron diffraction, Atomic Force Microscopy, Scanning Tunneling Microscopy, Spec-
Unit 4 Nanotechnology: Applications and Devices
Nanoscale materials, Nano transfer printing, Biomaterials applications, MEMS and NEMS, selforganisation, nanoscale (opto) electronics, Fullerenes, Devices - Actuators and motors for nanodisplacements, Nanosensors, development of optical memory using semiconductor nanoparticles - Nozzle-free in- kjet technology - Dendrimers and their application to organic electronics devices - Nanomedicines, Bio-imaging with quantum dots.

Unit 5 Environmental Issues in Nanotechnology
Nanoparticles and environment - Nanoparticles in atmosphere - Ground water, exhaust gases – wastewater and Indoor environments; Safety of nanoparticles - Problems caused by nanoparticles, Safety assessment for the nanoparticles; Removal of nanoparticles.

TEXTBOOKS:

REFERENCES:

18CHY637    MEDICINAL CHEMISTRY    3 0 0 3

Unit 1 Medicinal chemistry: Introduction, drugs – classification of drugs – mechanism of drug action. Drug- receptor complex, nomenclature – agonist,

Unit 2 Physicochemical properties of drugs in relation to biological action: solubility, Partition coefficient, dissociation constant, hydrogen bonding, ionization, drug shape, surface activity, complexation, protein binding, molar refractivity, bioisosterism – stereo chemical aspects of drug action.
Unit 2: Enzymes, hormones and Vitamins - representative cases, nomenclature, classification and characteristics of enzymes, mechanism of enzyme action, factors affecting enzyme action, co-factors and co-enzymes, enzymes in organic synthesis, mechanism of enzyme catalysis, enzyme inhibition. Hormones and vitamins – representative cases.

Unit 3 Essentials of drug design
Molecular mimetics, drug-lead modification, drug design using QSAR and computer assisted design, assessment of drug activity, receptors and drug action, mechanism of drug action, drug metabolism pathways, Drug potentiation, drug antagonism and drug resistance

Unit 4 Medicinal agents from natural products
History of the use of natural products as therapeutic agents, medicinal plants, active principle, Isolation methods of alkaloids, terpenes, antioxidants, natural oils from plants

Unit 5 Medicinal agents
Medicinal agents belonging to alkaloids, steroids, polypeptides, modified nucleic acid bases, sulphonamide and sulpha drugs, antibacterials - sulpha drugs, substituted sulphonamides, anticonvulsants, anticoagulants, antiamoebic agents, antihelmintic agents, anti-malarial agents, diuretics and cardio vascular agents, , medici-
nal agents affecting CNS, analgesics, antipyretics, antiseptics and disinfectants, Histamine and anti-histaminic agents. Infectious and non infectious diseases (malaria, AIDS, Cancer) introduction, mechanism of action types of cure,

**TEXTBOOKS:**

**REFERENCES**
2. V.K.Ahuwalia, Lalita S.Kumar and Sanjiv Kumar, ‘Chemistry of Natural Products’, Ane Books India.

**18CHY638 SUPRAMOLECULAR CHEMISTRY 3003**

**Unit 1 Introduction to Supramolecular Chemistry**
From molecular to supramolecular chemistry: Factors leading to strong binding, hydrogen bonding and stacking interactions, Bottom-up approach, Top-Down Approach, Energy and Signals Semiochemistry, photo switching devices, electro switching devices, mechanical switching processes.

**Unit 2 Processing of Energy and Signals by Molecular and Supramolecular system**
Fundamental principles of photo induced electron and energy transfer, Molecular electronics, Molecular photonics, Molecular Chemionics, Molecular electro photonics, Molecular Photochemionics.

**Unit 3 Molecular Recognition**

**Unit 4 Electrochemistry of Supramolecular Systems**
Electroluminescent systems as sensors and devices, Redox controlled molecular switches, Biohybrid electrochemical devices, Dendrimers as multielectron storage devices, Redox-active Metal-Polypyridinedendrimers as light harvesting antennae.

**Unit 5 Molecular Scale Mechanical Devices**
Introduction to mechanical devices, Spontaneous mechanical like motions, Allosteric movements, Tweezers and Harpoons, A natural proton pump, Twisters, Tweezers, Threading-Dethreading movements, Ring switching processes in Rotaxanes and Catenanes, Molecular valves, Molecular Muscles.

**TEXTBOOKS:**

**REFERENCES:**
**18CHY639 Nanomaterials for Biomedical Applications**

**Unit 1:** Introduction to Nanomaterials: Size dependence of properties – Surface to volume ratio and Quantum confinement. Microscopic techniques to study nano structures - SEM, AFM – TEM and STM. Spectroscopic techniques to characterize nanostructures - Raman, XPS, Auger, EDAX.

**Unit 2:** Synthetic approaches: Colloidal, Self-Assembly (Self assembled monolayers-SAMs) and electrostatic self-assembly, electrochemical methods (cathodic and anodic processes), sol-gel, Langmuir-Blodgett (LB) technique, chemical vapour deposition, plasma arcing and ball milling, lithography.

**Unit 3:** Electrical, optical, mechanical, chemical and magnetic properties of nanomaterials. Surface Plasmon resonance – Fluorescence Resonance energy transfer (FRET).

**Unit 4:** Carbon Clusters: Synthesis, properties and biomedical applications of Fullerenes, Carbon nanotubes and Graphenes. Quantum Dots, wells and wires (metallic and semiconducting) - Preparation, properties and biomedical applications. Dendrimeric structures and their applications.

**Unit 5:** Biofunctionalisation of nanomaterials - Noncovalent Assembly - Covalent assembly - Biofunctional Nanomaterials - Semiconductor Nanoparticles - Magnetic Nanoparticles. Applications of Biofunctional nanomaterials – Optical and Electrochemical Sensing.

**REFERENCES:**

**18CHY640 INDUSTRIAL METAL FINISHING PROCESSES**

**Unit 1** Background Theory: Review of reversible and irreversible processes - electrodes, indicator and reference - Nernst and Butler-Vohmer equation - phenomenon of polarization - factors influencing - Tafel experiment and Tafel plot - Significance.

**Unit 2** Electrodeposition: Industrial plating of copper-nickel (dull and bright) - chromium on mild steel – operating conditions and sequence – pre-treatment processes - plant layout – electroplating of zinc on MS and post plating chromating, yellow and blue passivation processes – decorative plating of silver and gold on non-ferrous metals – brief discussion on nano plating of metals and micro structure of the deposition. Properties of deposits: Tests for adhesion, hardness, thickness, uniformity and corrosion resistance of the electro deposits.

Electroless deposition: Nickel, copper, gold on metal components – bath composition and operating conditions - immersion plating - plating on plastics – pre-treatment processes – long duration plating – electroforming, operating conditions and sequence.

Nano anodizing of titanium, aluminium and tantalum – application to sensor field.

Plasma electrolytic oxidation: power supply requirements – baths used – process sequence for aluminium, magnesium and titanium – properties of the coating and industrial applications.

Unit 4 Electropolishing: Mechanism of electropolishing – electropolishing of ferrous and non-ferrous metals – industrial baths used – operating conditions and sequence - industrial applications.

Unit 5 Electrochemical etching: Etching of ferrous and non-ferrous metals – special properties of matt and satin finish – DC and AC processes – operating conditions and sequence.

Special Topics: Electrochemical and chemical metal colouring of ferrous and non-ferrous metals.


TEXTBOOK:

REFERENCES:

18CHY641 Biosensors : Fundamentals and Applications 3 0 0 3

Unit 1: Introduction to biosensor – classification based on the signal transduction and biorecognition element. Enzymatic and non-enzymatic sensors, DNA and protein based sensors-immunosensors.


Unit 4: Optical and electrochemical sensors for glucose, vitamins, cholesterol, dopamine, nitric oxide, nitrates, and pesticides. Biocompatibility of sensors.

Unit 5: Biochips and wearable devices: lab-on-a-chip - fabrication of microfluidics- lithography, wearable sensors, epidermal electronic system, lab-on-skin-devices.
REFERENCES


Unit 1 - Introduction

Introduction to computational chemistry (molecular modelling), questions commonly investigated computationally, principle and application of methods (tools) of computational chemistry - molecular mechanics, ab initio method, semiempirical methods, density functional theory and molecular dynamics, STOs, GTOs, basis sets, specification of molecular geometry using Cartesian coordinates and internal coordinates, Z-matrix, Z-matrix of simple molecules (water, ethanol), potential energy surface (PES), potential energy surface of diatomic molecules and triatomic molecules (H$_2$O and HOF) - hypersurface and process of “slicing”, stationary points on a potential energy surface - potential energy surface of the isomerization reaction of ozone to isoozone, stationary points (ozone, isoozone and transition state), intrinsic reaction coordinate, minimum, relative minimum, saddle-shaped surface, saddle point, higher-order saddle point and mathematical treatment of stationary points, Born-Oppenheimer approximation and its significance and frozen-nuclei energy.

Unit 2 - Molecular Mechanics

Introduction to molecular mechanics, forcefield, developing a force field - expression for potential energy of a molecule, bond stretching term, angle bending term, torsional term and nonbonded interaction term, parameterizing a forcefield - parameterizing bond stretching term, angle bending term, torsional term and nonbonded interaction term, calculation using forcefield - compare the energies of two 2, 2, 3, 3-tetramethylbutane geometries, illustration of application (use) of molecular mechanics - calculation of geometries and energies of small-sized and medium-sized molecules, polymers and transition states (transition state for the Diels-Alder reaction of butadiene with ethene to form cyclohexene), in organic synthesis for predicting the more suitable path for carrying out the synthesis and calculation of normal-mode vibrational frequencies for characterizing a species as a minimum or a transition state or higher-order saddle point, for obtaining zero-point energies to correct frozen-nuclei energies and for interpreting or predicting IR spectra, strength (merit) and weakness (demerit) of molecular mechanics.

Unit 3 - Semiempirical methods - Part 1

Introduction to semiempirical (SE) methods, Simple Huckel Method (SHM) - theory - expression for calculating energy of a molecular species, expression for molecular wave function based on LCAO approximation, secular equations and the single matrix equation, H, C, S and $\varepsilon$ matrices and their interpretation, the values of
H_{ij} as zero, coulomb integral \( \alpha \) and bond integral \( \beta \) and their physical significance, the H matrix in terms of \( \alpha \), \( \beta \) and zero for ethene system (ethene neutral molecule, ethene radical cation and ethene radical anion), propenyl system (propenyl cation, propenyl neutral radical and propenyl anion) and cyclobutadiene system (square cyclobutadiene dication, square cyclobutadiene neutral molecule and square cyclobutadiene dianion), the H matrix in terms of zero, \( \alpha = 0 \) and \( \beta = -1 \) for ethene systems (ethene neutral molecule, ethene radical cation and ethene radical anion), propenyl system (propenyl cation, propenyl neutral radical and propenyl anion) and cyclobutadiene system (square cyclobutadiene dication, square cyclobutadiene neutral molecule and square cyclobutadiene dianion), result of diagonalization of the H matrices written for ethene system, propenyl system and cyclobutadiene system, molecular orbital energy level diagrams and expressions for energy and molecular wave functions for ethene system, propenyl system and cyclobutadiene system based on the result of diagonalization of the H matrices, and molecular orbital energy level diagrams for ethene system, propenyl system and cyclobutadiene system showing ground state and excited state electronic configurations.

**Unit 4 - Semiempirical methods - Part 2**

Application of SHM - nodal properties of molecular orbitals and Woodward-Hoffmann orbital symmetry rule, stability towards oxidation and reduction of various species in ethene system, propenyl system and cyclobutadiene system, geometry of cyclobutadiene molecule as predicted by SHM and its Jahn-Teller distortion, aromaticity and Huckel’s \((4n + 2)\) \( \pi \) electron rule, and calculation of resonance (stabilizing) energy, bond order and atomic charges of various species in ethene system, propenyl system and cyclobutadiene system, strength of SHM, weakness of SHM (detailed explanation) - basis set is limited to p orbitals \((p_z)\), it treats only \( \pi \) electrons, and the overlap integrals, Fock matrix elements, electron spin and electron-electron repulsion are not calculated/accounted properly, Extended Huckel Method (EHM) - minimal valence basis set, calculation of Fock matrix elements, and calculation of overlap integrals by Lowdin orthogonalization, EHM procedure, EHM calculation on protonated helium molecule, application of EHM - an overall idea, strength and weakness of EHM, SCF SE methods - Pariser-Parr-Pople (PPP) method and Complete Neglect of Differential Overlap (CNDO) method - basic principle (an exhaustive treatment is not expected).

**Unit 5 - Density Functional theory and ab initio method**

(An exhaustive treatment is not expected)

Introduction to Density Functional theory and calculations, Kohn-Sham approach - the first and the second Hohenberg-Kohn theorems, introduction to ab initio method and calculation, basis sets for H, He and first, second and third row elements used in ab initio calculations - STO-3G, 3-21G, 3-21G(*) and 6-31G*, these basis sets for a few molecular species (water, methane and carbene), basic principles of ab initio method (an idea only).

**Text Book**

1. Computational Chemistry-Introduction to the Theory and Applications of Molecular and Quantum Mechanics - Errol Lewars

**18CHY643 Sustainable Chemical Science 3 0 0 3**

**Unit 1 Green Chemistry and Sustainability**

History of green chemistry, Chemical composition of the, environment (Air, water & soil- Role of organic and inorganic molecules in pollution), the twelve principles of green chemistry (detailed description with examples), green chemistry as an expression of environmental ethics (Thrift Chemistry), the concept of sustainability, from green to sustainable chemistry, sustainable use of chemical feedstock, water and energy,
quantifying greenness of a chemical reaction, green chemistry metrics- mass based, energy and environmental metrics, designing greener process, life cycle assessment (introduction and scope),Green toxicology- the need, principles of toxicology, Disposition of Toxicants in Organisms, Non-Organ System Toxicity, Mechanistic Toxicology, Quantitative Structure–Activity Relationships, (Environmental Toxicology-Persistence and bio-accumulation), Non-Cancer risk assessment, Cancer risk assessment, stakeholders in sustainable policy implementation.

Unit 2 Chemistry in water
Definition and attributes of a green solvent, the principle and reasons for use of water in green chemistry- hydrophobicity- cyclodextrin chemistry, Lewis acids in aqueous media, Michael addition in water using triflates, green processes with base in water, green oxidations and reduction in water, on water conditions, use of water in microwave and ultrasonic technology.

Unit 3 Green solvents
Ionic liquids as green solvents- definitionand notation- properties, synthesis and use in organic reactions, oxidation, oxidative carbonylation of aniline, Friedel–crafts reaction, Michael addition, Fischer Indole synthesis, Benzoin condensation, dimethyl carbonates synthesis in ionic liquids.


Properties and application in organic transformation of green solvents like polyethylene glycol, glycerol, cyclopentyl methyl ether, 2-methyltetrahydro furan, Perfluorinated (Fluorous) Solvents- FluorousBi-phase Concept and dimethyl carbonate.

Unit 4 Green Chemistry and Catalysis
Importance of catalysis, turn over number and frequency, the basis of catalysis-kinetic phenomenon, basics of homogeneous, heterogeneous and biocatalysis, sabatier’s principle, catalyst -deactivation, sintering, thermal degradation, inhibition and poisoning, catalyst promoters, modifiers, supported catalysts and reagents for green chemistry- heterogenized reactions for green chemistry, preparation of solid catalyst-slurry and co-precipitation, impregnation, hydrothermal synthesis- drying, calcination, activation and forming, selecting the right support, catalyst characterization- surface characterization methods, temperature programmed techniques, spectroscopy and microscopy.

Common mechanism in enzyme catalysis immobilized enzymes, developing biocatalyst- rational design and directed evolution, non-enzymatic biocatalysts.

Unit 5 Green Chemistry Technologies and Alternate Energy Sources
Design for Energy Efficiency, Photochemical Reactions Advantages of and Challenges Faced by Photo-chemical Processes (Examples)
Microwaves as energy source in chemistry- properties of microwaves, microwave heating (Effects), Approaches to Microwave-assisted Organic Chemistry- solvent free methods, MORE chemistry, continuous microwave reactor (CMR)-microwave batch reactor (MBR), examples of organic transformations.
Sonochemistry and Green Chemistry-Theoretical Basis- Cavitation Inception, Nucleation-Bubble Dynamics- examples of organic transformations, Sono-chemical synthesis of nano-structured materials,
Electrochemical Synthesis- materials manufactured using the process, organic electrosynthesis- 3-bromothiophen from thiophene

5. Handbook of Green Chemistry, Vol5 Green Solvents- Reactions in Water, PualT Anastas, Chao Jun Li

18CHY681 ORGANIC QUALITATIVE ANALYSIS LAB. 0 0 6 2

1. Separation of binary mixtures

Includes separation, preliminary investigations, determinations of saturation/unsaturation, detection of elements by Lassaigne’s test, functional group identification, derivative preparation, determination of melting points of the derivatives and calculation of Rf values from TLC

The following mixtures can be given:
(a) Acid and hydrocarbon
(b) Phenol and aldehyde
(c) Phenol and acid
(d) Phenol and amine
(e) Acid and ester
(f) Halo compound and aldehyde
(g) Acid and aldehyde
(h) Amine and aldehyde
(i) Amine and ketone
(j) Alcohol and hydrocarbon

2. Thin layer chromatography to determine Rf values of compounds
(a) 2-nitroaniline
(b) 4-nitroaniline
(c) Cinnamic acid and 2-nitroaniline
(d) Acetophenone
(e) Ethyl benzoate
3. Simple column chromatography to separate the components of binary mixtures
   (a) Hydrocarbon and ester
   (b) Aldehyde and amine

REFERENCES:

18CHY682 INSTRUMENTAL METHODS OF ANALYSIS LAB. 0 0 5 2

1. Determination of strengths of halides in a mixture potentiometrically.
2. To find the redox potential of the given sample using cyclic voltametry.
3. Determination of half wave potential of Cd & Zn by polarography.
4. Determination of pKa of an indicator in aqueous and micellar medium using UV-Vis spectroscopy.
5. Determination of stoichiometry and stability constant of inorganic (ferric-salicylic acid) and organic (aminoiodine) complexes using UV–Vis spectroscopy.
6. Determination of copper and cadmium in a mixture by electrogravimetry.
7. Determination of rate constant for enzyme kinetics-inversion of sucrose.

TEXTBOOKS:

REFERENCE BOOKS: