

DEPARTMENT OF CHEMISTRY
NORTH-EASTERN HILL UNIVERSITY
SHILLONG – 793022

M. Sc. CHEMISTRY SYLLABUS
CHOICE-BASED CREDIT SYSTEM
(APPROVED SYLLABUS: JUNE 2008)

INORGANIC CHEMISTRY - I**Unit 1 *Symmetry and Structure***

Symmetry elements and operations; equivalent symmetry elements and equivalent atoms; symmetry point groups with examples from inorganic compounds; groups of very high symmetry; molecular dissymmetry and optical activity; systematic procedure for symmetry classification of molecules and illustrative examples; molecular symmetry for compounds having co-ordination numbers 2 to 9.

Unit 2

(a) *Stereochemistry and Bonding*: LCAO-MO theory for homonuclear and heteronuclear diatomic molecules; orbital symmetry and overlap; Walsh diagrams; electronegativity (Pauling, Mulliken and Allred-Rochow methods); group electronegativity and polarity of bonds; review of VSEPR model and the use of outer d-orbitals

(b) *Metal-Ligand Equilibria in Solution*: Stepwise and overall formation constants; trends in stepwise formation constants; determination of binary formation constant by spectrophotometry; factors affecting stability of metal complexes and chelate effect.

Unit 3 *Magnetic Properties & Electronic Structure of Transition Metal Complexes*

Brief review of different types of magnetic behaviour, spin-orbit coupling, quenching of orbital angular momenta, temperature-independent paramagnetism, measurement of magnetic susceptibility using Gouy and Faraday methods, Term symbols for metal ions; Crystal field theory and its application to explain magnetic properties of coordination compounds, spin crossover; Structural effects: ionic radii and Jahn-Teller effect; octahedral vs. tetrahedral coordination, magnetic properties of Lanthanides and Actinides and splitting of f-orbitals in octahedral field.

Unit 4 *Electronic Structure of Transition Metal Complexes*

Electronic absorption spectra of octahedral and tetrahedral complexes, Orgel diagrams, Tanabe-Sugano diagrams, calculation of Dq , B and β values, selection rules, band intensities and band widths, spectra of high-spin octahedral and tetrahedral complexes of d^1 to d^9 systems, Spectrochemical series; Adjusted crystal field theory, Nephelauxetic series, molecular orbital theory of complexes (qualitative principles involved in complexes with and without π -bonding), MO diagrams for octahedral and tetrahedral complexes and charge-transfer spectra, optical properties of Lanthanides and Actinides.

Unit 5 *Organometallic Chemistry*

Synthesis, structure, bonding and reactivity of transition metal complexes with olefins, cyclopentadienyl, cyclopentadienide, benzenoid, π -allyl and enyl systems; Transition metal-carbon σ -bond: metal-alkyls, metal-carbenes, metal-carbynes.

Text Books

1. J. E. Huheey, E. A. Keiter, R. L. Keiter & O. K. Medhi. *Principles of Structure and Reactivity* (1st impression), Pearson Education (2006).
2. F. A. Cotton. *Chemical Applications of Group Theory*, (3rd edn.), John Wiley & Sons (1999).

Reference Books

1. P. Atkins, T. Overton, J. Rourke, M. Weller & F. Armstrong, *Shriver and Atkins Inorganic Chemistry*, Oxford University Press (2006).
2. N. N. Greenwood & A. Earnshaw. *Chemistry of the Elements*, Pergamon Press (1984).
3. F. Basolo & R. G. Pearson, *Mechanism of Inorganic Reactions*, Wiley Eastern (1967).
4. F. A. Cotton, G. Wilkinson, C. A. Murillo & M. Bochmann. *Advanced Inorganic Chemistry* (6th edition), John Wiley (1999).
5. S. F. A. Kettle, *Physical Inorganic Chemistry*, Spectrum (1996).
6. B. Douglas, D. McDaniel and J. Alexander. *Concepts and Models of Inorganic Chemistry* (3rd edn.), John Wiley & Sons (1994).

First Semester

Che C 102

Credits: 4

ORGANIC CHEMISTRY – I

Unit 1 Stereochemistry

Configuration nomenclature; Axial and planar chirality and helicity; Topicity and prostereoisomerism; Racemic modification and optical purity; Conformational analysis of acyclic, cyclic, heterocyclic and steroidal systems; Effects of conformation on reactivity; Regioselectivity, stereospecificity and stereoselectivity; Asymmetric synthesis (including enzymatic and catalytic nexus); Enantio- and diastereoselective synthesis.

Unit 2

(a) Nucleophilic Substitution Reactions: Nucleophilic substitution at saturated carbon – SN1, SN2 and related mechanisms; Parameters influencing reaction rates; Neighboring group participation by π and σ bonds, Anchimeric assistance; Synthetic applications of nucleophilic substitution involving alcohols, thiols, amines and hydrides; Aromatic nucleophilic substitutions.

(b) Structure and Reactivity: Linear free energy relationships, Hammett and Taft equations, σ and ρ parameters; Applications of acid-base concept, HSAB theory; Aromaticity in benzenoid and non-benzenoid compounds, antiaromaticity and homoaromaticity; Huckel rule, n-annulenes, heteroannulenes, fullerenes, cryptates.

Unit 3

(a) Elimination Reactions: Mechanism and stereochemistry of different types of elimination reactions; Effects of substrate structure, attacking base, leaving group and medium; Formation of other double bonds (C=N, C=O) and triple bonds by elimination reactions; Mechanism and orientation in pyrolytic elimination.

(b) Addition to Carbon-Carbon Multiple Bonds: Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals; Regio- and chemoselectivity; Orientation and reactivity; Addition to cyclopropane and carbon-heteroatom multiple bonds; Hydroboration, alkylation, epoxidation and hydroxylation; Addition of halogen polar reagents to alkenes.

Unit 4

(a) Carbonyl and Related Groups: Reactivity of carbonyl group, 1,3-dithiane reactivity, Umpolung effect; Ring expansions; Homologation and dehomologation of carbonyl compounds; Nucleophilic addition of hetero-atoms (N,O,S); Conjugate addition reactions, Acylation of carbonyl carbon; Carbonyl cyclizations and cleavages; Carboxylic acids and derivatives, decarboxylation reactions.

(b) Photochemistry: Photochemistry of alkenes and carbonyl compounds; Photooxygenation; Photochemistry of aromatic compounds; Photochemical isomerisation, addition and substitution; Photo-Fries rearrangement of ethers and anilides; Barton reaction, Hoffmann-Loeffler-Freytag reaction, di- π -methane rearrangement; Singlet molecular oxygen reactions; Photo-cleavages.

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Unit 5 *Pericyclic Reactions*

Main features of pericyclic reactions; Woodward-Hoffman rules, correlation diagram and FMO approaches; Electrocyclic reactions – conrotatory and disrotatory motions for $4n$ and $4n+2$ systems; Cycloadditions – antarafacial and suprafacial additions, [2+2] and [4+2] reactions ($h\nu$ and Δ), 1,3-dipolar cycloadditions and chelotropic reactions; Sigmatropic $[i,j]$ shifts of C-H and C-C bonds; Sommelet-Hauser, Claisen, thio-Claisen, Cope and aza-Cope rearrangements.

Text Books

1. S. H. Pine. *Organic Chemistry* (5th edn.), McGraw-Hill Book (1987).
2. J. March. *Advanced Organic Chemistry: Reactions, Mechanisms and Structure* (4th edn.), Wiley Student Edition, John Wiley & Sons Asia Pte. Ltd. (2005).
3. P. S. Kalsi. *Stereochemistry, Conformation and Mechanism* (3rd edn.), John Wiley (1995).
4. C. Depuy & O. L. Chapman. *Molecular Reactions and Photochemistry*, Prentice-Hall of India (1975).

Reference Books

1. F. A. Carey & R. J. Sundberg. *Advanced Organic Chemistry*, Part A and B, 3rd edn. (1990).
2. Wamser & Harris, *Fundamentals of Organic Reaction Mechanisms*, John Wiley (1990).
3. R. B Woodward & R. Hoffman, *Conservation of Orbital Symmetry*; Verlag-Chemie/Academic Press (1970).
4. I. Fleming. *Frontier Orbital Theory and Organic Reactions*, John Wiley & Sons (1976).
5. A. P. Marchand & R. E. Lehr, *Pericyclic Reactions*, Academic Press (1977).

PHYSICAL CHEMISTRY – I**Unit 1 *General Principles of Quantum Mechanics***

Introduction; operators and related theorems; uncertainty principle; postulates; properties of wave functions; Schrodinger equation; energy eigenvalue equation; equation of motion and constant of motion.

Unit 2 *Application to Simple Systems and Approximation Methods*

Exactly solvable problems: Particle in a box, harmonic oscillator, rigid rotator, step potential and tunneling, hydrogen atom.

Linear and non-linear variations method; applications (He atom and other simple systems); Hellmann-Feynmann theorem; antisymmetry principle and many-electron wave functions.

Unit 3 *Chemical Binding*

Born-Oppenheimer approximation; valence bond (VB) and molecular orbital (MO) theory for diatomic molecules – hydrogen molecule ion, hydrogen molecule; excited states of H₂ – singlet and triplet; non-crossing rule and correlation diagram; hybridization; Huckel MO treatment for simple and conjugated polyenes.

Unit 4 *Adsorption and Aggregation*

Surface tension and surface free energy; Pressure across an interface: Laplace equation, Kelvin equation; Wetting: Young-Dupre equation; Adsorption in liquid systems: Gibbs adsorption isotherm; Adsorption on solids: Langmuir isotherm, BET isotherm.

Surfactants, classification of surfactants, hydrophobic interaction, aggregation/micellization of surfactants, critical micelle concentration (cmc), factors affecting the cmc, thermodynamics of micellization: phase separation and mass action models.

Unit 5 *Solid State Chemistry-I*

Solid State Reactions: Types; sintering; nucleation; Factors influencing the reactivity of solids; Precursors to solid state reactions; Tammann and Hedvall mechanism; Wagner's diffusion theory of reaction; Material transport in solid state reaction—counter diffusion, Kirkendall effect; Huttig's mechanism; Kinetic model: Reaction in powder compact, parabolic rate law, Jander's rate equation.

Crystal Defects: Types of defects, thermodynamics of Schottky and Frenkel defect formation, Kroger-Vink notation for crystal defects

Atomic theory of diffusion—self diffusion mechanism.

Text Books

1. I. N. Levine. *Quantum Chemistry*, Prentice Hall India (2001).
2. D. A. McQuarrie. *Quantum Chemistry*, Viva Books Pvt Ltd (2003)
3. A. K. Chandra. *Introductory Quantum Chemistry*, Tata McGraw Hill (1994).
4. Y. Moroi. *Micelles: Theoretical and Applied Aspects*, Plenum (1992).
5. A. R. West. *Solid State Chemistry and its Applications*, John Wiley (1998).

Reference Books

1. P. W. Atkins. *Molecular Quantum Mechanics*, Oxford University Press (1986)
2. R. McWeeny. *Coulson's Valence*, ELBS (1979).
3. N. B. Hannay. *Solid State Chemistry*, Prentice-Hall (1979).
4. D. K. Chakraborty. *Solid State*, New Age International, New Deldi (1996).

First Semester**Che C 104****Credits: 6****LABORATORY COURSE – I
(ORGANIC CHEMISTRY)**

1. Purification Techniques of organic compounds and their spectroscopic identifications.
 - a) Purification of binary mixtures by Thin Layer Chromatography (TLC) and Column chromatography (CC).
 - b) Purification of tertiary mixtures of amino acids by Paper Chromatography.
2. Extraction of Natural Products: Any one of the following – solasodine, caffeine, nicotine, piperine, rosine, carotenoids.
3. Organic Preparations: At least eight preparations (involving two or more than two steps) involving the following representative reactions-
 - a. Esterification and saponification
 - b. Oxidation (peracid, chromic acid, Mn(VII))
 - c. Hydride reduction or hydrogenation
 - d. Nucleophilic substitution
 - e. Cycloaddition reaction
 - f. Grignard reaction
 - g. Condensation reaction
 - h. Preparation of dyes
 - i. Aromatic electrophilic substitution
 - j. Heterocyclic synthesis
4. Qualitative Analysis of Binary Mixtures (only two)

Text Books

1. R. K. Bansal. *Laboratory Manual of Organic Chemistry* (3rd edn.), Wiley-Eastern (1994).
2. R. G. Brewster & W.E. Mcwedd. *Unitized Experimental Organic Chemistry* (4th edn.), East-West Press (1977).
3. A. I. Vogel. *Practical Organic Chemistry* (3rd edn.), Longman Group Ltd. (1973).

Reference Books

1. A. O. Fitton & R. K. Smallery. *Practical Heterocyclic Chemistry*
2. R.L. Shriner & R. C. Fuson. *Systematic Identification of Organic Compounds* (5th edn.), John Wiley & Sons (1964).

Second Semester

Che C 201

Credits: 2

INORGANIC CHEMISTRY - II**Unit 1 *Homogeneous Catalysis***

Coordinative unsaturation, oxidative addition reactions, insertion reactions; Reactions of coordinated ligand and activation of small molecules by complexation; Catalytic reactions of alkenes: isomerization, hydrogenation, hydroformylation, hydrosilylation and polymerization.

Unit 2 *Transition Metal π -acid Complexes and Supramolecular Chemistry*

Bonding, synthesis and reactivity of transition metal complexes with CO, NO, O₂, N₂ and tertiary phosphine and arsine ligands; metal carbonyl hydrides and metal carbonyl clusters: LNCC and HNCC, Wade's rule and the capping rule.

Supramolecular chemistry: Definition, supramolecular host-guest compounds, macrocyclic effect, nature of supramolecular interactions.

Unit 3 *Kinetics and Mechanism of Inorganic Reactions*

Labile and inert complexes; mechanisms of ligand-replacement reactions; ligand displacement reactions in square planar and octahedral complexes; the *trans* effect; isomerisation and racemisation of tris-chelate complexes; electron transfer reactions; stereochemical nonrigidity and fluxional molecules.

Text Books

1. J. E. Huheey, E. A. Keiter, R. L. Keiter & O. K. Medhi, *Principles, Structure and Reactivity* (1st impression), Pearson Education (2006).
2. F. A. Cotton, G. Wilkinson, C.A. Murillo & M. Bochmann, *Advanced Inorganic Chemistry* (6th edn.), John Wiley (1999).

Reference Books

1. P. Atkins, T. Overton, J. Rourke, M. Weller & F. Armstrong. *Shriver and Atkins Inorganic Chemistry*, Oxford University Press (2006).
2. T. Moeller. *Inorganic Chemistry: A Modern Approach*, John Wiley (1982).
3. J. W. Steed & J. L. Atwood. *Supramolecular Chemistry*, John Wiley (2002).

ORGANIC CHEMISTRY – II

Unit 1 Reductive Reactions

(a) *Catalytic hydrogenation*: Scope and mechanisms for heterogeneous catalytic hydrogenation of alkenes and other functional groups; Reduction selectivity; Catalyst poisoning and desulphurization; Homogeneous catalytic hydrogenation with Wilkinson catalyst; Alkene double bond isomerisation.

(b) *Dissolving metal reductions*: Scope and basic mechanisms; Liquid ammonia reduction with alkali metals, Birch reduction of arenes; Acyloin condensation and related reactions.

(c) *Metal hydride reductions*: Scope, stereochemistry and mechanism of metal hydride reductions of carbonyl compounds; Reduction of other functional groups like nitro, nitroso, azo and oxime groups; MPV reduction; Use of hydroboration in reduction, oxidation and carbonylation, regioselectivity, stereo-selectivity and synthetic utility of alkyl boranes.

(d) *Reduction with hydrazine & derivatives*: Reduction of carbonyl group with hydrazine; *p*-tosylhydrazine, diimide and semicarbazide; Use of hydrazine with other reducing agents on conjugated systems.

Unit 2 Oxidation Reactions

(a) *Cr and Mn Oxidations*: Oxidation of alcohols & aldehydes with Cr(VI) & Mn(VII) oxidants; Oxidation of C=C and C-H bonds; Uses of PCC, PDC and Collin's reagent.

(b) *Peroxy Oxidations*: Alkene epoxidation by peracids and metal/alkyl hydroperoxides.

(c) *Other methods of oxidation*: DMSO and Swern oxidations; Oppenauer oxidation; Prevost and Woodward hydroxylation of alkenes; Oxidative cleavage of C-C single and double bonds; periodates, LTA, oxidation of organic substrates with mercuric acetate and SeO₂.

Unit 3 Reactive Intermediates

(a) *Carbenes*: Stability, structure and spin states of carbenes; Cyclopropanation – spin dependence and stereochemistry; Carbene insertion to C-H bonds; Rearrangement to alkenes; Wolff rearrangement of acylcarbenes and its synthetic applications; Carbenoids.

(b) *Nitrenes*: Stability, structure and spin states of nitrenes; C-H bond insertions and aziridine formation; Rearrangement of acylnitrenes (Hoffmann, Curtius and Schmidt reactions with applications in organic synthesis); Nitrenoids.

(c) *Free Radicals*: Stability and fate of organic free radicals; Metal-induced radical reactions; Radical cyclisation and coupling reactions; Addition to multiple bonds; Aromatic substitution by radicals; Allylic bromination by NBS and decarboxylative bromination; Mechanism of well-known radical reactions.

Textbooks

1. H. O. House. *Modern Synthetic Reactions*, W. A. Benjamin (1972).
2. J. March. *Advanced Organic Chemistry: Reactions, Mechanisms and Structure* (4th edn.), Wiley Student Edition, John Wiley & Sons Asia Pte. Ltd. (2005).
3. T. L. Gilchrist & C. W. Rees, *Carbenes, Nitrenes and Arynes*, Nelson, London (1969).
4. V. K. Ahluwalia & R. Aggarwal, *Organic Synthesis: Special Techniques*, Narosa Publishing House, New Delhi (2001).

Second Semester

Che C 203

Credits: 2

PHYSICAL CHEMISTRY – II**Unit 1 Microwave, Infrared and Raman Spectroscopy**

Introduction: Interaction of light with matter, mechanism of absorption & emission of radiation.

Microwave spectroscopy: Classification of molecules; rigid rotor model; rotational spectra of diatomics and polyatomics; effect of isotopic substitution and nonrigidity; selection rules and intensity distribution.

Vibrational spectroscopy: Vibrational spectra of diatomics; effect of anharmonicity; Morse potential; Vibration-rotational spectra of diatomics; P,Q,R branches, normal modes of vibration, overtones, hot bands.

Raman spectroscopy: Origin; rotational and vibrational Raman spectra of diatomics.

Unit 2 Electronic Spectroscopy

Electronic spectroscopy: Electronic spectra of diatomic molecules, Franck-Condon principle, Vibronic transitions, Spectra of organic compounds, $\pi \rightarrow \pi^*$, $n \rightarrow \pi^*$ transition.

Photoelectron Spectroscopy: Basic principles, photoelectron spectra of simple molecules, X-ray photoelectron spectroscopy (ESCA), Auger electron spectroscopy.

Lasers: Laser action, population inversion, properties of laser radiation, examples of simple laser systems.

Unit 3 Magnetic Resonance Spectroscopy

Nuclear Magnetic Resonance: Nuclear spin and nuclear spin states in magnetic field, resonance phenomenon, relaxation processes, NMR line shapes and saturation, shielding and de-shielding of magnetic nuclei, chemical shift, spin-spin interactions, spectra of a two-spin system (A₂, AB and AX cases), ¹³C, ¹⁹F, and ³¹P NMR spectroscopy.

Electron Spin Resonance: Basic principles, factors affecting g values, hyperfine coupling, spin densities and McConnell relationship. Zero field splitting.

Text Books

1. C. N. Banwell and E. M. McCash. *Fundamentals of Molecular Spectroscopy*, 4th edn., Tata McGraw-Hill, New Delhi, 1994.
2. D. A. McQuarrie and J.D. Simon –Physical Chemistry, VIVA Students Ed. (2003)

Reference Books

1. J. D. Graybeat. *Molecular Spectroscopy*, McGraw-Hill International Edition (1988).

Second Semester**Che C 204****Credits: 6**

LABORATORY COURSE – II
(INORGANIC CHEMISTRY)

1. Quantitative estimation involving volumetric (redox and complexometry), gravimetric and spectrophotometric methods of constituents in three component mixtures and alloys
2. Preparation and Characterization of the following compounds (at least 8 preparations are to be completed by turn):
 1. Reinecke salt
 2. Tris(oxalate) manganese(III)
 3. Tetrapyridinesilver(II)peroxodisulphate
 4. Tris(acetylacetonato) iron(III)
 5. Bis(N,N-diethyldithiocarbamate)nitrosyliron(I)
 6. Optical isomers of tris(ethylenediamine)cobalt(III)chloride
 7. Linkage isomers of nitro and nitritopentamminecobalt(III) chloride
 8. Ferrocene or dibenzene chromium
 9. Hydrido-chloro-carbonyl tris(triphenylphosphine)ruthenium(II)
 10. Tris(2,2'-bipyridine)ruthenium(II) perchlorate
 11. [(p-cymene)RuCl₂]₂
 12. Tri(acetylacetonato)manganese(III)
3. Characterization includes microanalysis, magnetic susceptibility and conductance measurements and infrared, UV-Visible, NMR spectroscopy and cyclic voltammetry studies

Text Books

1. J. Mendham, R. C. Danney, J. D. Barnes & M. Thomas. *Vogel's Textbook of Quantitative Chemical Analysis*, Peterson Education (2000).
2. G. Marr & B. W. Rockett. *Practical Inorganic Chemistry*, Van Nostrand (1972).
3. G. Pass & H. Sutcliffe. *Practical Inorganic Chemistry* (2nd edn.), Chapman & Hill (1974)

Reference Books

1. J. Basset, R. C. Denney, G.H. Jeffery & J. Mendham. *Vogel's Text Book of Quantitative Analysis* (4th edn.), English Language Book Society (1978).
2. H. H. Willard, L. L. Merrit & J. A. Dean. *Instrumental Methods of Analysis* (4th edn.), East-West Press (1974).
3. G. W. Parshall (Ed. in Chief). *Inorganic Synthesis*, Vol. 15, McGraw Hill, p. 48 (1974).

Third Semester

Che C 301

Credits: 2

INORGANIC CHEMISTRY–III

Unit 1

(a) Infrared and Raman Spectroscopy: Structural studies (involving IR and Raman spectroscopy) of coordination compounds containing the following molecules/ions and ligands - NH_3 , H_2O , OH^- , SO_4^{2-} , CN^- , SCN^- , NO , O_2 , PR_3 and halides.

(b) Magnetic Resonance Spectroscopy

Electron spin resonance spectroscopy: ESR of d^1 and d^9 transition metal ions in cubic and tetragonal ligand fields; evaluation of g values and metal hyperfine coupling constants.

Nuclear magnetic resonance spectroscopy: Applications of ^{31}P , ^{19}F , ^{119}Sn and ^{195}Pt NMR spectroscopy in the structural assessment of inorganic compounds.

Unit 2

(a) X-ray Crystallography: Lattices, planes and indices; X-ray diffraction and Bragg's law; Crystal systems and symmetry, point groups, stereographic projection of 32 point groups and space groups; Symmetry elements: isogonal symmetry groups and reciprocal lattice. Crystal growing; Data collection, data reduction, refinement and structure solution of some compounds

(b) Mossbauer Spectroscopy: Principles, isomer shift, quadrupole effect of magnetic field, applications to iron and tin compounds.

Text Books

1. K. Nakamoto. *Infrared and Raman Spectra of Inorganic and Coordination Compounds*, (5th edn.), John Wiley (1997).
2. R. V. Parish. *NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry*, Ellis Horwood, New York (1990).

Reference Books

1. R. S. Drago. *Physical Methods in Chemistry*, Saunders College Publishers (1977).
2. C. N. Banwell & E. M. McCash. *Fundamentals of Molecular Spectroscopy*, Tata McGraw-Hill, New Delhi (2006).

Third Semester**Che C 302****Credits: 2****ORGANIC CHEMISTRY – III****Unit 1**

(a) **Infrared Spectroscopy:** Characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols, amines; Detailed study of vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters, amides, acid anhydrides, lactones, lactams, conjugated carbonyl compounds); Effects of H-bonding and solvent effect on vibrational frequency, extension to various organic molecules for structural assignment.

(b) **Mass Spectroscopy:** Mass spectral fragmentation of organic compounds, common functional groups; molecular peak, McLafferty rearrangements, examples of mass spectral fragmentation of organic compounds with respect to their structure determination.

Unit 2

(a) **Nuclear Magnetic Resonance Spectroscopy:**

Approximate chemical shift values of various chemically non-equivalent protons and correlation to protons bonded to carbon (aliphatic, olefinic, aldehydic and aromatic); Protons bonded to other nuclei (alcohols, phenols, enols, carboxylic acids, amines, amides, SH); Chemical exchange, effect of deuteration; complex spin-spin interaction between two, three, four and interacting nuclei (first order spectra); Complex interaction, virtual coupling, stereochemically hindered rotation, Karplus curve, variation of coupling constant with dihedral angle, nuclear magnetic double resonance, simplification of complex spectra using shift reagents, Fourier transform technique and nuclear Overhauser effect (NOE).

(b) **C-13 NMR Spectroscopy:**

Chemical shift (aliphatic, olefinic, alkynes, aromatic, hetero-aromatic, carbonyl carbon); Coupling constants, two-dimensional NMR spectroscopy, NOESY, DEPT and INEPT terminologies.

(c) **Applications** of IR, NMR and Mass spectroscopy for structure elucidation of organic compounds.

Textbooks

1. R. M. Silverstein, G. C. Basseler & T. C. Morill. *Spectroscopic Identification of Organic Compounds*, John Wiley (1981).
2. W. Kemp. *Organic Spectroscopy* (3rd edn.), McMillan Press Ltd. (1991).

References

1. D. Williams & I. Fleming. *Spectroscopic Methods in Organic Chemistry*, McGraw Hill (1989).
3. C. N. Banwell & E. M. McCash. *Fundamentals of Molecular Spectroscopy*, Tata McGraw-Hill, New Delhi (2006).

Third Semester**Che C 303****Credits: 2****PHYSICAL CHEMISTRY – III****Unit 1 *Chemical Thermodynamics***

Introduction; Thermodynamics of open systems; Chemical potential; Definition of fugacity, standard state of real gases, the relation between fugacity and pressure; Partial molar quantities, partial molar volume and its determination, thermodynamics of mixing; Activity and activity coefficients.

Unit 2 *Statistical Thermodynamics*

Different types of ensembles, ensemble averaging, distribution law (Boltzmann statistics), partition function and thermodynamic parameters; relation between molecular and molar partition functions, translational partition function, rotational partition function for linear and non-linear molecules; vibrational partition function, electronic partition function, reference state of zero energy for evaluating partition function, equilibrium constant in terms of partition function.

Application of statistical thermodynamics: equipartition theorem, heat capacity behaviour of crystals.

Introduction to quantum statistics: Distribution law for fermions (Fermi-Dirac statistics) and for bosons (Bose-Einstein statistics).

Unit 3 *Non-Equilibrium Thermodynamics*

Entropy of irreversible processes – Clausius inequality; entropy production (heat flow, chemical reactions, electrochemical reactions) and entropy flow; Entropy production in open systems; Rate of entropy production – generalized forces and fluxes; Phenomenological equations, Onsager reciprocity relation; Electrokinetic phenomena; Stationary non-equilibrium states - states of minimum entropy production.

Text Books

1. P. W. Atkins & J. de Paula. *Physical Chemistry* (8th edn.), OUP (2006).
2. D. A. McQuarrie. *Statistical Mechanics*, Viva Books Pvt. Ltd., New Delhi (2003)
3. C. Kalidas and M. V. Sanganarayana. *Non-Equilibrium Thermodynamics – Principles and Applications*, Macmillan India (2002).

Reference Books

1. I. Prigogine. *Introduction to Thermodynamics of Irreversible Processes*, Interscience (1960).

Third Semester**Che C 304****Credits: 6****LABORATORY COURSE – III
(PHYSICAL CHEMISTRY)**

Students are to perform twelve experiments from the following list:

1. Determination of order of reaction, rate constant and energy of activation for saponification of an ester by NaOH, conductometrically.
2. Determination of strength of strong and weak acids in a mixture, conductometrically.
3. Determination of critical micellar concentration (CMC) of sodium lauryl sulphate from the measurement of conductivities at different concentrations.
4. Determination of strengths of halides in a mixture, potentiometrically.
5. Determination of pH of buffer solutions and hence to calculate the E₀ of quinhydrone electrode.
6. Determination of stoichiometry and formation constant of silver-ammonia complex, potentiometrically.
7. Verification of Beer-Lambert's law and determination of pK_a of an indicator, spectrophotometrically.
8. Spectrophotometric determination of pK_a of an indicator in micellar and microemulsion media.
9. Absorption spectra of conjugated dyes. Application of particle in a box model
10. Determination of partial molar volume of a solute in solution.
11. To study the complex formation between Ni Ions and 1,10-Phenanthroline.
12. Determination of the stability constant of the complex formed between Cu(II) ions and 5-sulphosalicylic acid between pH 3-5 by colorimetric method and hence to calculate the free energy of formation of the complex.
13. Determination of specific rotation of sucrose and rate constant of its hydrolysis using a polarimeter.
14. Determination of coordination number of Cu²⁺ in copper-ammonia complex by partition method.
15. Determination of solubility product of a sparingly soluble salt (PbSO₄, BaSO₄ etc.) conductometrically and verification of Debye-Huckel theory.
16. To study the kinetics of iodination of acetone.
17. To study the kinetics of a second order reaction (saponification of ethyl acetate).
18. Determination of the acidic and basic dissociation constants of an amino acid and hence its isoelectric point.

Textbooks

1. D. P. Shoemaker, C. W. Garland & J. W. Nibler. *Experiments in Physical Chemistry* (5th edn.), McGraw Hill (1989)
2. V. D. Athawala & P. Mathur. *Experimental Physical Chemistry*, New Age International Publishers (2001).

Fourth Semester**Che C 401****Credits: 4****INORGANIC CHEMISTRY - IV****Unit 1 *Bioinorganic Chemistry of Alkali and Alkaline Earth Metals***

Essential and trace elements in biological systems, structure and functions of biological membranes; mechanism of ion transport across membranes; sodium pump; ionophores: valinomycin and crown ether complexes of Na⁺ and K⁺; ATP and ADP; photosynthesis: chlorophyll a, PS I and PS II; role of calcium in muscle contraction, blood clotting mechanism and biological calcification.

Unit 2 *Bioinorganic Chemistry of Iron and Copper*

Iron-sulphur proteins: rubredoxin and ferredoxins; Metalloporphyrins; Heme proteins: hemoglobin, myoglobin and cytochrome c; Non-heme proteins: hemerythrin and hemocyanin; Nitrogen fixation and nitrogenases

Unit 3 *Photochemistry of Metal Complexes and Metal–Metal Multiple Bonds*

Excited states, ligand field states, charge-transfer states and Thexi states; Phosphorescence and fluorescence; Photochemical reactions: substitution and redox reactions of Cr(III), Ru(II) and Ru(III) complexes; Applications: synthesis and catalysis, chemical actinometry and photochromism; Metal-metal multiple bonds, major structural types, quadrupole bonds and one-dimensional solids.

Unit 4 *Nanomaterials*

General introduction to nanomaterials and emergence of nanotechnology; Moore's law; synthesis of nanoparticles of gold, rhodium, palladium, platinum, and silver; Synthesis of nanoparticle semiconductors, nanowires and nanorods; Techniques of synthesis: electroplating and electrophoretic deposition, conversion through chemical reactions and lithography; Thin films: Chemical vapor deposition and Atomic layer deposition techniques; Carbon fullerenes and nanotubes. Applications of nanoparticles.

Unit 5 *Selected Topics*

Synthesis, properties and structures of boranes, carboranes, silicones, phosphazenes and S,N compounds; isopolyacids and hetero-polyacids; non-stoichiometric oxides: zeolites and clay; polymorphism of carbon, phosphorus and sulphur; thermal methods of analysis (TGA, DTA and DSC).

Text Books

1. R. C. Mehrotra & A. Singh. *Organometallic Chemistry: A Unified Approach* (2nd edn.), New Age International (2000).
2. F. A. Cotton & G. Wilkinson. *Advanced Inorganic Chemistry* (5th edn.), John Wiley (1988)
3. D. M. Roundhill. *Photochemistry and Photophysics of Metal Complexes*, Plenum Press (1990).
4. G. Zhong Cao. *Nanostructures and Nanomaterials: Synthesis, Properties and Applications*, Imperial College Press (2004).
5. G. H. Stout & L. H. Fensen. *X-ray Structure Determination: A Practical Guide*, Macmillan (1968).

Reference Books

1. C. Cotal & A. W. Adamson, *Comprehensive Coordination Chemistry*, Vol. 1, Editor-in-Chief G. Wilkinson (1985).
2. A. W. Adamson & P. D. Fleischauer. *Concepts of Inorganic Photochemistry*, John Wiley & Sons (1975).
3. M. Ratner & D. Ratner. *Nanotechnology: A Gentle Introduction to the Next Big Idea*, Pearson Education (2003).
4. P. Atkins, T. Overton, J. Rourke, M. Weller & F. Armstrong. *Shriver and Atkins Inorganic Chemistry*, Oxford University Press (2006).

ORGANIC CHEMISTRY – IV

Unit 1

(a) **Introduction:** Hantzsch-Widman nomenclature for monocyclic, fused and bridged heterocycles; General approaches to heterocyclic synthesis; Aliphatic and aromatic heterocycles; Basicity and aromaticity of heterocycles.

(b) **Small Ring Heterocycles:** Syntheses of aziranes, oxiranes & thiiranes; Ring openings and heteroatom extrusion; Synthesis & reactions of azetidines, oxetanes & thietanes; Strain.

Unit 2

(a) **Azoles:** Structural and chemical properties; Synthesis of pyrazole, isothiazole and isoxazole; Synthesis of imidazoles, thiazoles & oxazoles; Nucleophilic and electrophilic substitutions; Ring cleavages; Benzofused analogues.

(b) **Condensed Five-membered Rings (1 Heteroatom):** Synthesis of indole, benzofuran and benzo-thiophene; Nucleophilic, electrophilic and radical substitutions; Addition reactions; Indole rings in biology.

Unit 3

(a) **Diazines:** Structural & chemical properties; Synthesis of pyridazines, pyrimidines, pyrazines; Nucleophilic and electrophilic substitutions.

(b) **Bicyclic Heterocycles:** Synthesis of quinolines, isoquinolines, benzofused diazines, acridines, phenothiazines, carbazoles and pteridines; Substitution reactions.

(c) **Seven-membered Rings:** Synthesis & reactions of azepines, oxepines, thiepinines & diazepines

Unit 4

(a) **Porphyrins:** Classification and synthesis of porphin rings; Natural and synthetic metalloporphyrins; importance in biology.

(b) **Biological Heterocycles:** Chemical and biological properties and total synthesis of thiamine, lysergic acid, reserpine, nicotine, phenanthrene alkaloids, papaverine, nucleic acids bases.

Unit 5

(a) **Nucleic Acids:** Primary, secondary and tertiary structure of DNA; DNA replication and heredity; Structure and function of mRNA, tRNA and rRNA.

(b) **Proteins:** Acid-base properties of amino acids; polypeptides; primary, secondary, tertiary and quaternary protein structures; classification of proteins on basis of structure and biological function; Merrifield peptide synthesis.

Textbooks

1. L. A. Paquette. *Modern Heterocyclic Chemistry*, W. A. Benjamin (1968).
2. I. L. Finar. *Organic Chemistry*, Vol. II, ELBS (1986).
3. T. L. Gilchrist. *Heterocyclic Chemistry*, Longman (1989).
4. A. L. Lehninger. *Biochemistry*, Kalyani Publishers (1983).

Reference Book

1. A. R. Katritzky & C. W. Rees. *Comprehensive Heterocyclic Chemistry*, Vols. 1-7, Pergamon Press (1984).

PHYSICAL CHEMISTRY – IV

Unit 1 Reaction Kinetics-I

Determination of rate laws: Integral, isolation, half-life and differential methods; comparison of different techniques.

Kinetic equations for complex reactions: Chain, parallel, opposing and consecutive reactions; Enzyme catalysis.

Experimental verification: Flow, stopped-flow, Relaxation and NMR techniques.

Unit 2 Reaction Kinetics-II

Theory of reaction rates; Temperature effect on reaction rates; Rate constant for simple bimolecular reactions; Collision theory; Activated complex theory.

Reactions in solutions: Diffusion controlled & activation controlled reactions; Thermodynamic formulation of rate constant: effect of pressure & ionic strength.

Reaction in surfaces: Langmuir adsorption isotherm; kinetics of surface catalyzed unimolecular & bimolecular reactions; Applications in ammonia synthesis and oxidation of carbon-monoxide.

Unit 3 Electrochemistry-I

Ion-solvent interaction: free energy change due to ion-solvent interactions; Born model; electrical double layer; Helmholtz-Perrin model; Gouy-Chapman diffuse charge model and Stern model.

Electrodics: The basic electrodic equation: Butler-Volmer equation; overpotential; polarizable and nonpolarizable interfaces.

Unit 4 Electrochemistry-II

Ion-ion Interaction: Debye-Huckel theory of ion-ion interaction; Linearized Poisson-Boltzmann equation; ion-cloud and chemical potential change; activity coefficients and mean ionic activity coefficients; expression of mean ionic activity coefficients in terms of ionic strength.

Unit 5 Solid State Chemistry-II

Solid Solutions: Substitutional, interstitial and substitutional solid solutions & distortions.

Metals, insulators and semiconductors; Electronic structure of solids—band theory; intrinsic and extrinsic semiconductors, p-n junction.

Superconductors—Meissner effect, BCS theory.

Electrically conducting organic solids: Organic charge-transfer complexes, organic metals

Textbooks

1. K. J. Laidler, *Chemical Kinetics* (4th Edn.), Pearson Education (2007).
2. J. O'M Bockris and A. K. N. Reddy. *Modern Electrochemistry*, Plenum, New York (1970).
3. A. R. West. *Solid State Chemistry and its Applications*, John Wiley (1990).

Reference Book

1. M. J. Pilling and P. W. Seakins. *Reaction Kinetics*, NP (1995).

Second Semester**Che O 201****Credits: 2****MEDICINAL CHEMISTRY-I****Unit 1 Introduction**

Concept of drug, lead compound and lead modification, prodrugs and soft drugs; Structure-activity relationship (SAR), quantitative structure-activity relationship (QSAR); Factors affecting bioactivity – resonance, inductive effect, isosterism, bio-isosterism, spatial considerations; Theories of drug activity – occupancy theory, rate theory, induced fit theory
Concept of drug receptors – elementary treatment of drug-receptor interactions; Physico-chemical parameters – lipophilicity, partition coefficient, electronic ionization constants, steric, Shelton and surface activity parameters and redox potentials; Factors affecting modes of drug administration, absorption, metabolism and elimination; Significance of drug meta-bolism in medicinal chemistry.

Unit 2 Antibiotics

Cell wall biosynthesis, inhibitors of β -lactam rings, antibiotics inhibiting protein synthesis; Isolation, structure elucidation, synthesis, SAR and mode of action of penicillins; Synthesis of penicillin G, penicillin V, ampicillin, amoxicillin and cephalosporin.

Isolation, structure elucidation, synthesis, SAR and mode of action of following antibiotics: streptomycin, tetracyclines and chloroamphanicol.

Text Books

1. Burger. *Medicinal Chemistry and Drug Discovery*, Vol-1, Ed. M. E. Wolff, John Wiley (1994).
2. Goodman & Gilman. *Pharmacological Basis of Therapeutics*, McGraw-Hill (2005).
3. S. S. Pandeya & J. R. Dimmock. *Introduction to Drug Design*, New Age International.(2000).
4. D. Lednicer. *Strategies for Organic Drug Synthesis and Design*, John Wiley (1998).
5. Graham & Patrick. *Introduction to Medicinal Chemistry* (3rd edn.), OUP (2005).

Second Semester

Che O 202

Credits: 2

TOPICS IN ORGANIC SYNTHESIS

Unit 1 Reaction, Mechanism and Applications

(a) *Nucleophilic C-C bond formation*: Henry reaction, Wittig reaction and Horner-Wordworth-Emmons reaction and their selectivities; Chemistry of enolates – *E,Z* geometry of enolates, kinetic vs thermodynamic control of enolates, stereoselective enolate reactions, alkylation, aldol condensation (Zimmerman and Evans models), Mukaiyama reaction.

(b) *Electrophilic C-C bond formation*: Nazarov cyclization, Prins reaction, Vilsmeier-Hack reaction, Pictet-Sprengler reaction, reactions of π -allyl palladium complexes, Heck reaction, Stille coupling, Noyori reaction, reactions of allylsilane.

(c) *Miscellaneous reactions*: Biginelli reaction, Hantzsch reaction, Passerini reaction, Ugi reaction, McMurry olefination, Suzuki coupling, Ring closing metathesis (RCM) - Grubb's reaction, Mitsunobu reaction, Nef reaction, Sharpless asymmetric epoxidation and asymmetric dihydroxylation.

(d) *Arynes*: Generation, structure and stability of arynes; Benzyne mechanism for aromatic nucleophilic substitution; Direction of aryne bond formation and of nucleophilic addition; Rearrangement and cyclo-addition reactions of arynes; Trapping of arynes.

Unit 2 Reagents in Organic Synthesis

Use of following reagents/reactions in organic synthesis and functional group transformations: K-selecteride and L-selecteride, sodium cyanoborohydride, super hydrides, 9-BBN, IBX, Dess-Martin periodinane, manganese dioxide, Fetizon reagent, dioxiranes, ceric ammonium nitrate, Gilman's reagent, lithium diisopropylamide, dicyclohexylcarbodiimide, trimethylsilyl iodide, tri-*n*-butyltin hydride, Tebbe reagent, Corey-Nicolaou reagent, Peterson's synthesis, baker's yeast, lipase, Mosher's reagent, use of Os, Ru, and Tl reagents and DDQ.

Text Books

1. F. A. Carey & R. J. Sundberg. *Advanced Organic Chemistry Part B*, Plenum Press (2007).
2. M. B Smith. *Organic Synthesis* (2nd end.), McGraw-Hill, Inc. (2001).
3. J. March. *Advanced Organic Chemistry: Reactions, Mechanism and Structure* (4th edn.), John Wiley & Sons (2005).

Reference Books

1. W. Carruthers. *Some Modern Methods of Organic Synthesis* (4th edn.), Cambridge University Press (2004).
2. B. M Trost & I Fleming. *Comprehensive Organic Synthesis*, Vols 1-9, Pergamon (1991).

Second Semester**Che O 203****Credits: 2****COMPUTER PROGRAMMING IN CHEMISTRY****Unit 1 *Introduction to FORTRAN Language and Programming***

Constants, variables and expressions, input and output statements, format specifications, control statements, nesting of loops, arrays and subscripted variables, functions and subroutines.

Unit 2 *Numerical Analysis*

Data fitting by least square, Newton–Raphson and iterative methods for solving non-linear equations; Linear simultaneous equations - Cramer’s rule, Gauss elimination method and Gauss-Seidel method; Numerical integration – interpolation, Gauss’s quadrature formula; trapezoidal method, Simpson’s 1/3 rule.

Unit 3 *Practicals*

On-hand practical training with computers on selected chemical problems based on the numerical techniques of Unit 3.

Text Books

1. W. E. Mayo & M. Chiakala. *Programming with FORTRAN 77*, Schaum’s Outline Series, New Delhi (1995).
2. E. Balagurusamy. *Computer Oriented Statistical and Numerical Methods*, Macmillan India Ltd. (1988).
3. A. C. Norris. *Computational Chemistry: An Introduction to Numerical Methods*, John Wiley, New York (1981).

Reference Books

1. E. Kreyszig. *Advanced Engineering Mathematics* (5th edn.), Wiley Eastern Ltd. (1985).
2. C. Xavier. *Programming in Fortran 77 and Numerical Methods*. Asian Books (1998).

Second Semester

Che O 204

Credits: 4

ORGANOMETALLIC CHEMISTRY

Unit 1 *Main Group Organometallics*

Synthesis and reactions of organolithium compounds; Synthesis and reactions of organo-magnesium compounds; Organometallics of zinc and mercury: preparation, structure, bonding and reactions of aluminum organyls; Thallium(I) organyls (synthesis of TICp); Organyls of sodium, synthesis of NaCp; Silicon and tin organyls of coordination number 4.

Unit 2 *Transition Metal–Carbon Bond*

(a) *Transition Metal–Carbon σ -Bond*: Brief review of metal alkyl compounds; transition metal-carbene and transition metal-carbyne compounds; transition metal vinylidene and transition metal allenylidene compounds.

(b) *Transition Metal–Carbon π -Bond*: Cyclopropenyl cation ($C_3R_3^+$) as a ligand; C_4R_4 as a ligand (R = H, Me, Ph)

Unit 3 *Syntheses of Cyclopentadienyl and Arene Metal Analogues*

Synthesis and reactions of cyclopentadienyl metal carbonyls, cyclopentadienyl metal hydrides, cyclopentadienyl metal halides, arene metal carbonyls, η^6 -arene-chromium tricarbonyl in organic synthesis.

Unit 4 *Applications to Organic Synthesis and Homogeneous Catalysis*

(a) *In Organic Synthesis*: Hydrozirconation of alkenes and alkynes; Carbonylation of Colman's reagent; η^4 -diene iron-tricarbonyls in organic synthesis

(b) *In Catalysis*: Asymmetric hydrogenation; synthesis of acetic acid and glycol (Monsanto acetic acid process); Arylation/vinylation of olefins (Heck reaction); Wacker process (olefin oxidation); Asymmetric epoxidation.

Text Books

1. C. Elschenbroich. *Organometallics* (3rd edn.), Wiley-VCH Publication (2006).
2. C. Elschenbroich & A. Salzer. *Organometallics – A Concise Introduction* (2nd edn.), VCH Publication (1992).
3. F. Mathey & A. Sevin. *Molecular Chemistry of the Transition Elements*, John Wiley (1996).
4. F. A. Cotton & G. Wilkinson. *Advanced Inorganic Chemistry* (5th edn.), John Wiley (1988).
5. R. C. Mehrotra & A. Singh. *Organometallic Chemistry: A Unified Approach* (2nd edn.), New Age International (2000).

Reference Books

1. Yamamoto, *Organo Transition Metal Chemistry*, Wiley (1986).
2. R. H. Crabtree, *The Organometallic Chemistry of the Transition Metals* (4th edn.), John Wiley (2005).
3. A. J. Pearson. *Metallo-Organic Chemistry*, John Wiley & Sons (1985).
4. M. Bochmann. *Organometallics-1 Complexes with Transition Metal–Carbon σ -Bonds*, Oxford Chemistry Primers (1994).
5. M. Bochmann. *Organometallics-2 Complexes with Transition Metal–Carbon π -bonds*, Oxford Chemistry Primers (1994).

Second Semester

Che O 205

Credits: 4

BIOORGANIC CHEMISTRY**Unit 1**

Cell structure and metabolism: Prokaryotic and eukaryotic cells; Intracellular organelles and their functions; Comparison of plant and animal cells; Metabolic processes – catabolism and anabolism; ATP – currency of biological energy; Energy-rich and energy-poor phosphates.

Carbohydrates: Structure and function of sugar derivatives (deoxy, amino, branched chain sugars); Polysaccharides of biological importance, dextran, sialic acid; Cell-cell recognition and blood group substances.

Unit 2 Metabolic Reactions

Fatty acid metabolism: Biological importance of fatty acids and lipids, even chain and odd chain fatty acids, saturated and unsaturated fats, ketone bodies, fatty acid metabolism, calorific value of foods, biological membranes, properties and function of lipid bilayers and liposomes.

Protein-related transformations: Amino acid degradation (C3, C4, C5 family), urea cycle, uric acid and ammonia formation; Enzymatic hydrolysis of proteins to peptides; Amino acid sequencing; amino acid metabolism (biosynthesis and degradation).

Unit 3 Nucleic Acids

Chemical and enzymatic hydrolysis of nucleic acids; Structure and function of mRNA, tRNA, rRNA; Polymorphic nature of DNA, B- and Z-DNA, multi-stranded DNA; DNA sequence determination by chemical and enzymatic methods, Genetic code – origin, salient features, wobble hypothesis; Gene expression – transcription and translation; Gene mutation and carcinogenesis

Unit 4 Enzymes and Co-Enzymes

(a) Co-enzyme chemistry: Cofactors derived from vitamins, coenzymes, prosthetic groups, apoenzymes; Structure & biological function of coenzyme A, thiamine pyrophosphate, pyridoxal phosphate, NAD⁺, NADP⁺, FMN, FAD, lipoic acid and vitamin B12; Mechanisms of reactions catalyzed by above co-factors.

(b) Enzyme models: Host-guest chemistry, chiral recognition and catalysis, molecular recognition, diometric chemistry, crown ether, cryptates; Cyclodextrins, cyclodextrin-based enzyme models, calixarenes, ionophores, micelles, synthetic enzymes.

Textbooks

1. Stryer, L. *Biochemistry* (4th edn.), W. H. Freeman & Co. (1995).
2. Zubay, S. *Biochemistry*, Addison-Wesley (1983).
3. Sindell, R. P. *DNA Structure and Function*, Academic Press (1994).
4. Saenger, W. *Principles of Nucleic Acid Structure*, Springer-Verlag (1984).

Reference Books

1. Gringauz, A. *Introduction to Medicinal Chemistry: How Drugs Act and Why?* John Wiley & Sons (1997).
2. Dugas, H. & Penny, C. *Bioorganic Chemistry: A Chemical Approach to Enzyme Action*, Springer Verlag (1998).

Continued

3. Palmer, T. *Understanding Enzymes*, Prentice Hall (1995).
4. M.I. Page and A. Williams (eds.). *Enzyme Mechanisms*, Royal Society of Chemistry, (1987).
5. Price, N. C. & Stevens, L. *Fundamentals of Enzymology*, Oxford University Press (1989)
- 6 Trevan, M. D. *Immobilized Enzymes: An Introduction and Applications Biotechnology*, John Wiley (1980).
7. Fersht, A. & Freeman, W. H. *Enzyme Structure and Mechanism*, W.H. Freeman, New York (1985).
- 8 Metzler, D. E. *Biochemistry: The Chemical Reactions of Living Cells*, Academic Press (2001)

Second Semester

Che O 206

Credits: 4

CHEMISTRY OF SURFACTANTS**Unit 1 Introduction**

(a) Characteristic Features of Surfactants: General structural features & behavior of surfactants, classification of surfactants, hydrophobic/solvophobic interaction, Kraft point.

(b) Adsorption of Surfactants: Adsorption at solid/liquid, liquid/gas and liquid/liquid interfaces, Gibbs adsorption equation, adsorption isotherms, effect of added electrolyte on the surface excess of ionic surfactants.

Unit 2 Micelles

Micelle formation by surfactants: Critical micelle concentration, cmc measurement, conductance behaviour of ionic micellar solution, micellar structure and shape, factors affecting cmc, temperature dependence of cmc, thermodynamics of micellization, counterion binding constant.

Unit 3 Mixed Surfactants

Different types of mixed micelle, cmc of mixed micelle, Clint's equation for cmc, Rubingh's treatment, Rodenas treatment, counterion binding in mixed surfactants.

Unit 4 Solubilisation and Emulsification

Solubilization and Emulsification by Surfactants: Factors determining extent of solubilization, formation of emulsions, factors determining emulsion stability, microemulsions, conductance behaviour of microemulsions, reactions in micellar and microemulsion media.

Text Books

1. M. J. Rosen. *Surfactants and Interfacial Phenomena* (3rd edn.), John Wiley (2004).
2. Y. Moroi. *Micelles*, Plenum (1992).

Reference Books

1. K. R. Lange. *Surfactants*, Hanser Pub. (1999).
2. R. Zana (ed.). *Dynamics of Surfactant Self-Assemblies*, CRC Press (2005).
3. M. Abe & J. F. Scamehorn. *Mixed Surfactant Systems*, CRC Press (2004).

Second Semester**Che O 207****Credits: 4****SOLID STATE CHEMISTRY****Unit 1 *Solid State Reactions***

Preparative Methods: Vapor phase transport, preparation of thin films - electrochemical methods, chemical vapour deposition; Crystal growth - Bridgman & Stokbarger methods, zone melting. Characterization of Solids: Crystal diffraction of X-rays, X-ray diffraction method; Powder method – principles and uses; Scattering of X-rays by crystals – systematic absences; Electron diffraction; Neutron diffraction.

Unit 2 *Powder Compact Reactions and Solid-State Defects*

Diffusion Model: Parabolic rate law, Jander's rate equation, Kroger-Zeigler equation, Ginstling-Brounshtein rate equation.

Stoichiometric Defects: Equilibrium concentration of point defects in crystals - Schottky defects, Frenkel defects; The photographic process - light sensitive crystals, mechanism of latent image formation, lithium iodide battery.

Non-Stoichiometric Defects: Origin of non-stoichiometry, consequences of non-stoichiometry; Equilibria in non-stoichiometric solids, Color centers: F-centre, electron and hole centre; colour centre and information storage.

Unit 3 *Solid Electrolytes*

Typical Ionic Crystals: Alkali metal halides (vacancy conduction), silver chloride (interstitial conduction); Solid Electrolytes - β -alumina, silver iodide, halide and oxide ion conductors; Application of Solid Electrolytes. Fuel cells: electrochemical power generator (hydrogen-oxygen cell, Solid state Galvanic cell); Thermoelectric Effects: Seebeck effect; Hall Effect.

Unit 4 *Magnetic and Optical Properties of Solids*

Behaviour of substances in magnetic field; Effects of temperature (Curie & Curie-Weiss laws); Magnetic moments; Mechanism of ferro- and antiferromagnetic ordering – super exchange.

Luminescence and phosphors; Configurational coordinate model, Antistoke phosphors, Lasers — ruby and neodymium.

Conducting Organics: Organic conductors, preparation, mechanism of conduction in organic semiconductors, photoconductivity of polymers.

Text Books

1. A. R. West. *Solid State Chemistry and its Applications*, John Wiley (1987).
2. F. Gutmann & L.E. Lyons. *Organic Semiconductors*, John Wiley (1987).
3. N. B. Hannay, *Solid State Chemistry*, Prentice Hall of India (1979)

Reference Books

1. L. I. Buguslavski & A. V. Vannilov. *Organic Semiconductors and Biopolymers*, Plenum Press (1988).
2. R. J. D. Tiley. *Defect Crystal Chemistry and its Applications*, Chapman and Hall, New York (1987).
3. E. J. W. Whittaker. *Crystallography*, Pergamon Press Oxford (1981).

Second Semester**Che O 301****Credits: 2****ENVIRONMENTAL AND ANALYTICAL CHEMISTRY****Unit 1 *Air and Water Pollution***

Air pollution – types and sources; Atmospheric chemistry, depletion of stratospheric ozone, industrial and transport-related air pollution; Global warming and its effects.

Water pollution – types and sources, physical and chemical water pollutants, waste water treatment, criteria of water quality.

Unit 2 *Electrochemical and Spectral methods*

Polarography: Principle, instrumentation and applications, Cyclic voltammetry, Anodic stripping voltammetry, Amperometry, Coulometry and Conductance methods; Potentiometry: Ion selective electrodes; Atomic absorption spectrometry; Atomic fluorescence spectrometry; Turbidimetry and Nephelometry.

Unit 3 *Experimental Techniques of Purification and Separation*

Solvent extraction: principles of extraction, percentage extraction, action of ion exchange resin, ion exchange equilibria, applications.

Liquid chromatography: adsorption and partition chromatography, exclusion chromatography, HPLC (principles, equipment, choice of mobile phase and detector, column efficiency, applications.

Gas chromatography: Principles, instrumentation, choice of column and detector, applications .

Text Books

1. A. K. De. *Environmental Chemistry* (4th edn.), New Age International Limited (2006).
2. P. M. S. Monk. *Fundamentals of Electroanalytical Chemistry*, John Wiley & Sons (2001).
3. H. H. Willard, L.L. Merritt, J.A. Dean & F. A. Settle. *Instrumental Methods of Analysis* (7th edn.), Wadsworth Publishing Company, California (1988).
4. J. Mendham, R. C. Denney, J. D. Barnes and M. Thomas. *Vogel's Textbook of Quantitative Chemical Analysis*, Peterson Education (2000).

Reference Books

1. J. W. Moore & E. A. Moore. *Environmental Chemistry*, Academic Press, London (1976).
2. I. Pulford & H. Flowers. *Environmental Chemistry at a Glance*, Blackwell Publishing (2006).
3. S. E. Manahan. *Environmental Chemistry* (6th edn.), Lewis Publishers, London (1994).

Third Semester**Che O 302****Credits: 2****MEDICINAL CHEMISTRY-II****Unit 1 Drug Types - I**

(a) *Antineoplastic drugs*: Cancer chemotherapy, role of alkylating agents and antimetabolites in the treatment of cancer; Carcinolytic antibiotics and mitotic inhibitors; Synthesis of mechlorethamine, melphalan, 5-bromouracil and 6-mercaptopurine; Anticancer action of cisplatin and taxol.

(b) *Cardiovascular drug*: Classification, synthesis and mode of action of quinidine, verapamil, methyldopa and buphenine.

(c) *Hypnotics and sedatives*: SAR and mode of action; Synthesis of diazepam, oxazepam, chlorazepam, alprazolam, barbiturates, thiopental sodium.

(d) *Local anaesthetics*: Classification, SAR and mode of action; Synthesis of procaine, α -eucaine and β -eucaine, xylocaine, cinchocaine and quinisocaine.

Unit 2 Drug Types - II

(a) *Antiinfective drugs*: Mode of action and synthesis of sulphonamides, furazolidone, ciprofloxacin, norfloxacin, daspone, isoniazide.

(b) *Antipyretic Analgesics*: Classification and mode of action of antipyretic analgesics; Synthesis of paracetamol, chincophan, Novalgin and mefenamic acid.

(c) *Antihistamines*: SAR and mode of action of H₁-receptor antagonists; Synthesis of bromazine, mepyramine, methapyriline, antazoline, promethazine and phenindamine.

(d) *Antimalarial drug*: Nitrogen heterocycles as antimalarial agents, their classification and mode of action, synthesis of chloroquine, pamaquine, primaquine, Mepacrine and pyrimethamine. Introductory idea on Artemisinin, artemether and arteether.

Text Books

1. Burger. *Medicinal Chemistry and Drug Discovery*, Vol-1, Ed. M. E. Wolff, John Wiley (1994).
2. Goodman & Gilman. *Pharmacological Basis of Therapeutics*, McGraw-Hill (2005).
3. S. S. Pandeya & J. R. Dimmock. *Introduction to Drug Design*, New Age International.(2000).
4. D. Lednicer. *Strategies for Organic Drug Synthesis and Design*, John Wiley (1998).
5. Graham & Patrick. *Introduction to Medicinal Chemistry* (3rd edn.), OUP (2005).

Third Semester**Che O 303****Credits: 2****PHOTOCHEMISTRY****Unit 1 *Physical Properties of Excited Molecules***

Nature of changes on electronic excitation, Potential energy diagram, Absorption band shape and Franck-Condon Principle, Emission Spectra, Environmental effects on absorption and emission properties, Excited state dipole moment, Redox potential and acidity constants of aromatic acids.

Unit 2 *Photophysical Processes in Excited State*

Types of photophysical pathways, Radiationless transitions, Fluorescence emission, Triplet state and phosphorescence emission, Fluorescence quenching, Stern-Volmer equation, Concentration quenching and excimer formation, Quenching by foreign substrates, Exciplex formation.

Unit 3 *Applications of Photochemistry*

Importance of photochemistry, origin of life, photosynthesis and mechanism of vision.

Text Books

1. C. E. Wayne & R. P. Wayne, *Photochemistry*, OUP (1996).
2. N. J. Turro. *Modern Molecular Photochemistry*, University Science Books (1991).

Reference Books

1. J.B. Buirks. *Photophysics of Aromatic Molecules*, Wiley-Interscience (1969).
2. A. Gilbert & J.E. Baggott, *Essentials of Molecular Photochemistry*, Blackwell Scientific, Oxford (1991).

BIOINORGANIC CHEMISTRY**Unit 1 *Scope of Bioinorganic Chemistry***

Inorganic elements in biological systems, cells, biologically important compounds amino acids, proteins, nucleotides, carbohydrates and lipids, basic bioenergetics, classification of enzymes.

Biochemistry: Distribution, biological roles, active transport of cations across membranes, the sodium pump, biology of calcium carriers, role in muscle contraction, enzyme stabilization, blood clotting and biological calcification

Unit 2 *Metalloporphyrins*

Structure and optical spectra; heme proteins: magnetic susceptibility, epr and electronic spectra; hemoglobin and myoglobin: molecular structures, thermodynamics and kinetics of oxygenation, electronic and spatial structures, synthetic oxygen carriers, model systems; iron enzymes, peroxidase, catalase and cytochrome P-450

Unit 3 *Metalloenzymes*

Copper enzymes, superoxide dismutase, cytochrome oxidase and ceruloplasmin; Coenzymes; Molybdenum enzyme: xanthine oxidase; Zinc enzymes: carbonic anhydrase, carboxy peptidase and interchangeability of zinc and cobalt in enzymes; Vitamin B12 and B12 coenzymes; Iron storage, transport, biomineralization and siderophores, ferritin and transferrins..

Unit 4 *Metals in Medicine*

Metal deficiency and disease; toxicity of mercury, cadmium, lead, beryllium, selenium and arsenic; biological defence mechanisms; chelation therapy; metals used for diagnosis and chemotherapy, platinum complexes as anticancer drugs, Pt-DNA binding, complexes of gold, copper, zinc, mercury, arsenic and antimony as drugs.

Text Books

1. S. J. Lippard & J. M. Berg. *Principles of Bioorganic Chemistry*, Panima Publ. Corpn. (2005).
2. E.-I. Ochiai. *Bioinorganic Chemistry – An Introduction*, Allyn and Bacon Inc. (1977).
3. M. N. Hughes. *The Inorganic Chemistry of Biological Processes*, Wiley (1981).
4. R.P. Hanzlik. *Inorganic Aspects of Biological and Organic Chemistry*, Academic Press (1976)

Reference Books

1. H. Kraatz & N. Metzler-Nolte (Eds.). *Concepts and Models in Bioinorganic Chemistry*, Wiley (2006).
2. I. Bertini, H. B. Gray, S. J. Dippard & J. S. Valentine, *Bioinorganic Chemistry*, Viva Books Pvt. Ltd. (2004).
3. A.W. Addison, W.R. Cullen, D. Dolphin & B.R. James (eds.). *Biological Aspects of Inorganic Chemistry*, John Wiley (1977).
4. R.J.P. Williams & J.R.R.F. Dasilva. *New Trends in Bioinorganic Chemistry*, Academic Press (1978).
5. A. E. Martel. *Inorganic Chemistry in Biology and Medicine*, ACS Symp. Series, ACS (1980).
6. S. J. Lippard. *Progress in Inorganic Chemistry: Bioinorganic Chemistry*, Vol. 38, John Wiley, (1990).
7. N. Kaim & B. Schwederski. *Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life*, John Wiley (1994).

NATURAL PRODUCTS CHEMISTRY**Unit 1 *Natural Products and their Biosynthetic Pathways***

General classification of natural products, their isolation and characterisation and biosynthesis of common plant products; Biosynthesis pathways for natural products using co-enzymes and enzymes; Synthesis of selected natural products based on genetic classification – fatty acid derivatives and related compounds, general biogenesis and synthesis of cis-jasmone, methyl jasmonate, prostaglandins, exaltone and muscone.

Unit 2 *Synthetic Strategies*

Synthons and synthetic equivalents, disconnection approach, functional group inter-conversions, importance of order of events in organic synthesis, one group and two group C-X disconnections, chemoselectivity, reversal of polarity, cyclisation reactions, amine synthesis.

One group C-C disconnections – alcohols and carbonyl compounds, regioselectivity, alkene synthesis, use of acetylenes and aliphatic nitro compounds in organic synthesis.

Two group C-C disconnections – Diels-Alder reaction, 1,3-difunctionalised compounds, α,β -unsaturated carbonyl compounds, control in carbonyl condensations, 1,5-difunctionalised compounds, Michael addition and Robinson annelation. Principle of protection of alcohol, amine, carbonyl and carboxyl groups; Common protecting groups; Retrosynthetic analysis; Synthesis of quercetin, pinene, camphor and emitine.

Unit 3 *Terpenoids and Alkaloids*

General biosyntheses of mono- and sesquiterpenes, *trans*-chrysanthemic acid, cyclo-pentato monoterpene lactones, Synthesis of α -vetivone and total synthesis of β -eudesmol; Synthesis of hirsutene, abietic acid, *cis* juvenile hormone; *trans* annular cyclisation of caryophyllene, synthesis of caryophyllene and isocaryophyllene; Rearrangements of santonic acid and thujospene; Synthesis and rearrangement of longifolene

Structure, synthesis and biosynthesis of common alkaloids: reticuline, yohimbine and tylophorine.

Unit 4 *Steroids*

Biosynthesis of diterpenes, higher terpenes and steroids; Nomenclature of steroids and synthesis of squalene; Lanosterol and caretonoids; Synthesis of equilenins; Estrogens and total synthesis of non-aromatic steroids (progesterones); Corticosteroids; Degradation of diosgenin to progesterone and its synthesis; Miscellaneous transformations of steroid molecules.

Textbooks

1. K. Nakanashi. *Natural Products Chemistry*, Vols. I and II, Academic Press, New York and London (1974).
2. M. Harmata. *Strategies and Tactics in Organic Synthesis 4 & 5*, Academic Press (2004)

Reference Books

1. T. L. Gilchrist. *Heterocyclic Chemistry* (2nd edn.), Longman Scientific & Technical Publicns. (1992).
2. R. K. Bansal. *Heterocyclic Chemistry: Synthesis, Reactions and Mechanisms*, Wiley Eastern (1991).

Third Semester**Che O 306****Credits: 4****PRINCIPLES AND APPLICATIONS OF FLUORESCENCE SPECTROSCOPY****Unit 1 Introduction**

Phenomenon of fluorescence: Jablonski diagram; characteristics of fluorescence emission - Stokes shift, mirror-image rule; lifetimes and quantum yields; Fluorescence quenching: mechanism & dynamics; Fluorescence anisotropy; Fluorescence standards

Unit 2 Solvent and Environmental Effects on Fluorescence

Solvent polarity effect; Derivation and application of Lipper-Mataga (LM) equation, effect of viscosity, temperature effects; Additional factors that effect fluorescence emission; effect of solvent mixtures: specific and non-specific interactions.

Biochemical applications of environment sensitive fluorescent probes.

Unit 3 Instrumentation for Fluorescence Spectroscopy

Spectrofluorimeters: light source, monochromator, optical filters, photomultiplier tube, polarizers; Time domain measurements: importance.

Basics of time correlated single photon counting, data collection, analysis based on non-linear least square (NLSS) and maximum entropy method (MEM).

Unit 4 Applications of Fluorescence Phenomena

Fluorescence sensing: Mechanism of sensing; sensing techniques based on (i) collisional quenching, (ii) energy transfer, (iii) electron transfer; examples of (i) pH sensors, (ii) glucose sensors & (iii) protein sensors.

Novel fluorophores: (i) quantum dots, (ii) lanthanides and (iii) long-lifetime metal-ligand complex; Radiative decay engineering – metal enhanced fluorescence; DNA technology – sequencing, high sensitivity DNA stains, DNA hybridization.

Text Books

1. B. Valeur. *Molecular Fluorescence: Principles and Applications*, Wiley-VCH (2001).
2. J. R. Lakowicz. *Principles of Fluorescence Spectroscopy*, Springer (2006).

Reference Book

1. D. L. Andrews & A.A. Demidov, *Resonance Energy Transfer*, John Wiley & Sons (1999).

Third Semester**Che O 307****Credits: 4****COMPUTATIONAL QUANTUM CHEMISTRY****Unit 1 *Many Electron Theory***

Indistinguishability of particles; Antisymmetry principle and many electron wave function; Hartree-Fock theory; Roothaan equations, Koopman's theorem; Population analysis; Basis set; Electron correlation.

Unit 2

(a) ***Radiation-Matter Interaction***: Time-dependent perturbation theory; semi-classical treatment of radiation-matter interaction; Transition probabilities and rates; Einstein's A and B coefficients, selection rules.

(b) ***Density Functional Theory***: Hohenberg-Kohn theorem; Kohn-Sham theory; exchange-correlation functionals

Unit 3 *Applications*

Potential energy surfaces; weak interactions; thermochemistry and kinetics of simple chemical reactions; spectroscopy

Unit 4 *Introduction to Chemical Reaction Dynamics*

Types of chemical reactions; Atom-diatom interaction; Harmonic oscillator model for diatom. The collinear arrangement- Hard sphere model; Reaction cross section and flux density.

Text Books

1. P. W. Atkins. *Molecular Quantum Mechanics*, Oxford Univ. Press (1986).
2. N. Szabo & S. Ostlund. *Quantum Chemistry*, ELBS (1979).
3. R. Wyatt. *Dynamics of Molecules and Chemical Reactions*, World Scientific (2000).

Reference Books

1. M. Baer. *Theory of Chemical Reaction Dynamics*, CRC Press (1985).
2. F. L. Pilar. *Elementary Quantum Mechanics*, Tata McGraw-Hill (1990).