

UM-DAE Centre for Excellence in Basic Sciences (CBS)
Syllabus for M. Sc. (Int.) Chemistry

First year
Semester I

Subject Code	Subject	Contact hrs/per week (Theory +tutorials)	Credits
M101	Mathematics I (Calculus)	2 + 1	3
P101	Physics I (Classical Physics)	2 +1	3
C101	Chemical I (Structure & Bonding)	2 + 1	3
B101	Biology I (Cell Biology etc.)	2 + 1	3
G101	Computer basics	2 + 1	3
H 101	Communication Skills	2 + 0	1
		Contact hrs/per week Lab	Credits
PL101	Physics Laboratory	3	2
CL101	Chemistry Laboratory	3	2
BL101	Biology Laboratory	3	2
GL101	Computer Laboratory	3	2

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C101: Structure and Bonding

(35 + 10 = 45 hrs.)

a. Structure and Properties of atoms:

(12 + 6 = 18 hrs.)

- i) Atomic spectra, Bohr's theory of atomic structure, Sommerfeld's theory for complex electron spin and magnetic quantum number, Pauli exclusion principle, Hund's rule, electron configuration of elements, Sequence of energy levels and Periodic Table.
- ii) Size of atoms and ions, ionization energy, electron affinity, electronegativity – values by Pauling, Mulliken and Allred-Rochow, Metallic character, variable valency and oxidation states, Standard electrode potentials and electrochemical series, occurrence and isolation of the elements, horizontal, vertical and diagonal relationships in the periodic table.
- iii) Atomic Nucleus: Fundamental particles, classification of nuclides – isotopes, isomers, isobers, stable and unstable nuclides, nuclear stability - Even-odd nature of the number of protons and neutrons, the neutron to proton ratio N/Z, nuclear potential, binding energy, exchange force. Radioactivity and radioactive elements, radioactive decay and decay kinetics.

b. Chemical Bonding:

(12+ 6 = 18 hrs.)

- (i). The covalent bond - the Lewis theory, Octet rule and its limitations. Shapes of the molecules – Sidgwick – powel theory. Valence shell electron pair (VSEPR) theory, effect of lone pair and electronegativity, isoelectronic principle, examples to apply VSEPR theory. Valence bond theory. Hybridization. Bond length, bond angle & dihedral angle, d-orbital participation in molecular bonding, sigma and pi bonding. Molecular orbital method – Linear combination of atomic orbitals (LCAO), MO treatment for di- and tri-atomic molecules and involving delocalized pi-bonding. Conjugation & aromaticity
- (ii) Metallic bond – general properties, crystal structures (cubic close packed, hexagonal close packed and body centered cubic), free electron theory, valence bond theory, MO or band theory, Conductors, insulators and semiconductors,

alloys, superconductivity. (iii) physical properties and molecular structures – polarizability and dipole moments, melting point, solubility and acid-base properties, Intermolecular forces (dipole-dipole interaction) Hydrogen bonding and vander Waals's forces.

c. Structure, Reactivity & Mechanism:

(6+3= 9 hrs)

- (i) Nomenclature of organic compounds, homologous series and major classes of organic compounds- aliphatic, aromatic, alicyclic and heterocyclic compounds. Inductive and field effects, bond angle, bond distance and bond dissociation energy. p-d bonding – ylides. Delocalization –cross conjugation, resonance. Aromaticity and Huckel's rule – systems of $4n$ and $4n+2$ electrons, antiaromaticity, y-aromaticity, homo-aromaticity n-annulenes, heteroannulene, . Resonance and Hyperconjugation. Keto-enol tautomerism, alternate and non-alternate hydrocarbons fullerenes, C-60, cryptates, addition compounds, inclusion compounds, crown ethers, cyclodextrins, catenanes and rotaxanes.
- (ii) Reaction mechanism: Structure and Reactivity: Types of mechanisms, types of reactions, thermodynamic and kinetic requirements, Hammond postulate, Curtin-Hammett principle, transition states and intermediates, methods of determining mechanisms, isotopic effects. Generation, structure, stability and reactivity of carbocations, carbanions, free radicals, carbenes and nitrenes. Effect of structure on reactivity. The Hammett equation and linear free energy relationship (sigma-rho) relationship, Taft equation. Stereochemistry and rearrangements.

Reference Books:

1. J.D.Lee, Concise Inorganic Chemistry, 4th Edition, ELBS, 1991.
2. P.W.Atkins, Physical Chemistry, Oxford University Press, 7th Edition, 2006.
3. G.M.Barrow, Physical Chemistry, 5th Edition, Tata McGraw-Hill, New Delhi, 1992.
4. D.A.McQuarrie and J.D. Simon, Physical Chemistry - a molecular approach, Viva Books Pvt. Ltd. (1998).
5. H. J. Arnikaar, Essentials of Nuclear Chemistry Wiley Eastern Ltd.

Semester II

Subject Code	Subject	Contact hrs/per week (Theory +tutorials)	Credits
M201	Mathematics II (Linear Algebra and calculus of several variables)	2 + 1	3
P201	Physics II (Modern Physics)	2 +1	3
C201	Chemistry II (Thermodynamics and Chemical equilibrium)	2 + 1	3
B201	Biology II (Molecular Biology)	2 + 1	3
G201	Electronics & Instrumentation	2 + 1	3
H 201	History of Science	2 + 0	1
		Contact hrs/per week Lab	Credits
PL201	Physics Laboratory	3	2
CL201	Chemistry Laboratory	3	2
BL201	Biology Laboratory	3	2
GL101	Electronics Laboratory	3	2

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C201: Chemistry II (Thermodynamics & Chemical Equilibrium) (30 + 15 = 45 hrs.)

a. Thermodynamics:

(18+ 9= 27 hrs.)

- (i) Basic concepts – concept of system, boundary and surroundings, Homogeneous and heterogeneous systems, isolated, closed, and open systems, intensive and extensive properties, equilibrium and nonequilibrium states, reversible and irreversible processes.
- (ii) Heat, work and energy, irreversible and reversible expansion work of an ideal gas, internal energy in a cyclic process.
- (iii) First law of thermodynamics, heat content or enthalpy of a system, molar heat capacities, Joule-Thomson effect, Adiabatic expansion of an ideal gas and work done.
- (iv) Thermochemistry – Enthalpy of a reaction, exothermic and endothermic reactions, thermochemical equation, Kirchoff's equation, heat of reaction and flame temperature, heat of combustion, heat of solution, heat of neutralization, heat of fusion, heat of vaporization, Bond energy and dissociation energy, Hess's law and its applications.
- (v) Second law of thermodynamics, Carnot cycle, entropy, entropy change and irreversible processes and Clausius inequality, entropy and available work, entropy and probability.
- (vi) Free energy functions and Maxwell's relations, Gibb's Helmholtz relations, criteria of spontaneity and conditions of equilibrium, Heat capacity relations (C_p/C_v and $C_p - C_v$), change of phase and Clapeyron equation, Trouton's rule.
- (vii) Nernst heat Theorem and third law of thermodynamics, experimental determination of entropy.

b. Chemical equilibrium

(12+ 6= 18 hrs.)

- i. Chemical equilibrium and chemical potential (μ): chemical potential of an ideal gas and gas mixture, Gibbs free energy and entropy of mixing, Chemical equilibrium in a

mixture of ideal gases and real gases, Equilibrium constants – K_x and K_c , Temperature dependence of equilibrium constant, equilibrium between ideal gases and pure condensed phase. Lechatelier principle and applications.

- ii. Phase equilibrium in simple systems: Equilibrium condition, stability of the phases of a pure substance, pressure dependence of μ vs. T curves, Clapeyron equations, Phase equilibrium: solid- liquid, liquid-gas, solid-gas, phase diagram – water, carbon dioxide, sulphur, Effect of pressure on the vapour pressure, the phase rule.
- iii. Ideal solutions and colligative properties: ideal solutions, chemical potential of a solute in a binary ideal solution – Gibbs-Duhem equation, Colligative properties – freezing point depression, solubility, elevation of boiling point, Osmotic pressure, Vant Hoff equation.
- iv. Chemical statistics: Thermodynamic probability, most probable distribution (Boltzmann), partition function and thermodynamic functions – internal energy, entropy, free energy, pressure, Gibbs potential, Heat content, heat capacity, molar partition function, The third law of thermodynamics, Partition function and translational, rotational and vibrational energy.

Reference Books:

1. P.W. Atkins, Physical Chemistry, Oxford University Press, 7th Edition, 2006.
2. G.W. Castellan, Physical Chemistry, 3rd Ed. Addison - Wesley/Narosa Publishing House, 1993.
3. G.N. Lewis and Randall, Thermodynamics, (Revised by K.S. Pitzer
4. and L. Brewer), International Students Edition, McGraw Hill, 1961.
5. D. R. Gaskell, Introduction to Metallurgical Thermodynamics.
6. K. Denbigh, The principles of Chemical Equilibrium.
7. B. G. Kyle, Chemical & Process Thermodynamics.
8. G. W. Castellan, Physical Chemistry, Narosa Publishing House.

SECOND YEAR

Semester III

Subject Code	Subject	Contact hrs/per week (Theory +tutorials)	Credits
M 301	Mathematical Methods	3 + 1	4
CB 301	Biochemistry	3 + 1	4
CB302	Chemistry of Inorganic Molecules I	3 + 1	4
G301	Statistical Techniques and Applications	3 + 1	4
H 301	World Literature	2 + 0	2
		Contact hrs/per week Lab	Credits
CBL301	Chemistry-Biology Laboratory	6	6
GL301	Applied Electronics Laboratory	3	3

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CB301 Biochemistry

(45 + 15 = 60 hrs.)

- 1) **Overview of Biochemistry:** The concept of pH, dissociation and ionization of acids and bases, pKa, buffers and buffering mechanism, Henderson Hasselbalch equation, dissociation of amino acids and determination of pKa.
- 2) **Cellular macromolecules** (*in details, a brush up of the basics may be necessary*): Amino acids and proteins, Carbohydrates, Nucleotides and nucleic acids, Lipids, Vitamins, Hormones
- 3) **Protein structure and function:** folding, modification, targeting & degradation, enzymes, enzyme kinetics, enzyme regulation and inhibition
- 4) **Metabolism and metabolic pathways:** Glycolysis, TCA cycle, Oxidative Phosphorylation, Photophosphorylation
- 5) **Biosynthesis of macromolecules:** Carbohydrate biosynthesis (Pentose phosphate pathway), Fatty acid synthesis, Cholesterol of steroid biogenesis, Amino acid biosynthesis & degradation, Nucleotide biosynthesis & degradation, Fatty acid degradation
- 6) **Biochemistry of signal transduction and of hormone action in both plants and animals.**

Recommended Reading:-

- a. Lehninger Principles of Biochemistry, Fourth Edition by David L. Nelson (Author), Michael M. Cox (Author).
- b. Stryer L (1995) Biochemistry, 4 th edition, W. H. Freeman & company, New York.
- c. Energy and Entropy equilibrium to stationary states, Starzak, Michael E. 2010, XI, 303 p.
- d. Fundamentals of General Organic and Biological Chemistry (Study Guide) by **John McMurry** (Paperback - Jan. 1999).

CB302: Chemistry of Inorganic Molecules I:

(45 + 15 = 60 hrs.)

CB 302: Chemistry of Inorganic Molecules I**(45 + 15 = 60 hrs.)**

- a) **Redox reactions:** Oxidation number and oxidation states, Oxidation – reduction reactions and the use of reduction potential.
- b) **Theory of acids and bases:** Bronsted acids and bases, gas phase vs. solution acidity, solvent levelling effects, hardness and softness, surface acidity.
- c) **Hydrogen:** Preparation of hydrogen, Isotopes, ortho and para hydrogen, hydrides.
- d) **Rare gases:** Occurance and recovery of the elements, physical and chemical properties, Clathrate compounds, chemistry of Xenon and xenon fluoride complexes.
- e) **Chemistry of s-block elements:** a) alkali and alkaline metals: Extraction, general physical properties, flame colours and spectra, Reaction with water, air and nitrogen, oxides, hydroxides, peroxides and superoxides, sulphides, oxysalts, halides and hydrides, organic and organometallic compounds, the chlor-alkali industry. b) Group IIB elements: Zn, Cd, Hg.
- f) **Chemistry of p-block elements:** a) Group IIIA elements: Boron, aluminium, gallium indium and thalium – physical properties, oxidation states and type of bonds, Reactions with other elements, compounds of boron with oxygen and hydrogen. b) Group IVA elements: carbon, silicon, germanium, tin and lead – physical properties, allotropes of carbon, graphite compounds, carbides, carbonates, carbon cycle, silicates, organosilicons, hydrides, halides and cyanides, cluster compounds. c) Group VA elements: Nitrogen, phosphorous, Arsenic, antimony and bismuth – general properties, hydrides, azides, oxides and oxyacids, sulphides and organometallics, fertilizers. d) Group VIA elements: oxygen, sulphur, selenium, tellurium and polonium – general properties, structure and allotropy of the elements, chemistry of ozone, oxides, oxyacids, oxohalides, hydrides and halides, organo derivatives. e) Group VIIA elements: Fluorine, chlorine, bromine, iodine and Astatine- general properties, oxidizing power, hydrogen halides, ionic and molecular halides, bridging halides, halogen oxides, oxoacids, interhalogen compounds, polyhalides, pseudohalogens and pseudohalides. f) Group IIB elements

Text / References:

1. J. E. Huheey, 'Inorganic Chemistry - Principles of Structure and Reactivity' Harper & Row, 1988.
2. F. A. Cotton and G. Wilkinson, 'Advanced Inorganic Chemistry', John Wiley, 1995.
3. D. F. Shriver, P.W. Atkins and C.H. Langford, 'Inorganic Chemistry', Oxford University Press, 1991.
4. M.V. Hughees, 'The Inorganic Chemistry of the Biological Processes',; John Wiley, 1981.
5. F. A. Cotton and G. Wilkinson, Basic Inorganic Chemistry, Wiley Easter, 1978.
6. M. J. Sienko and R.A. Plane, Chemical Principles and Properties, McGraw Hill, 1975.
7. J. D. Lee, Concise Inorganic Chemistry, Van Nostrand Reinhold, 1977.

**Second Year
Semester IV**

Subject Code	Subject	Contact hrs/per week (Theory + tutorials)	Credits
PCB401	Chemical kinetics and Reaction Dynamics	3 + 1	4
CB402	Chemistry of Organic Molecules I	3 + 1	4
PCB402	Atomic and Molecular Spectroscopy	3 + 1	4
CB404	Advanced Molecular Biology	3 + 1	4
G401	Energy & Environment	2 + 1	3
		Contact hrs/per week Lab	Credits
CBL401	Chemistry-Biology Laboratory	3	3
GL401	Computational Laboratory	3	3

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PCB401: Chemical Kinetics & Reaction Dynamics: (45 + 15 = 60 hrs.)

- i) **Basic Concepts:** Rate, order and molecularity of a reaction, First, second and third order reactions – effect of concentration on reaction rate, rate expressions and integrated form, pseudo-unimolecular and second order autocatalytic reactions, nth order reaction of a single component, effect of temperature on reaction rate – Arrhenius equation and activation energy.
- ii) **Complex Reactions:** parallel first order reactions, series first order reactions – determination of rate constants by graphical method and the time ratio method. The stationary state, radioactive decay, general first order series and parallel reactions. Competitive, consecutive second order reactions, reversible reactions, equilibrium from the kinetic view point, complex mechanisms involving equilibria.
- iii) **Kinetic Measurements:** Experimental determination of reaction rates and order of reactions – correlation of physical properties with concentrations, reactions in the phase, reactions at constant pressure, fractional-life period method, initial rate as a function of initial concentrations.
- iv) **Reactions in Solutions:** General Properties, Phenomenological theory of reaction rates, Diffusion limited rate constant, Slow reactions, Effect of ionic strength on reactions between ions, Linear free energy relationships, Relaxation methods for fast reactions.
- v) **Catalysis:** Homogeneous catalysis in gas phase, in solution, basis of catalytic action, catalysis and the equilibrium constant, acid base catalysis, The Bronsted catalysis law, linear free energy changes, general and specific catalysis. Heterogeneous catalysis. Negative catalysis and inhibition, Surface reactions – effect of temperature and nature of surface. Industrial catalysis.
- vi) **Chain reactions:** general treatment, activation energy, chain length, chain transfer reactions, inhibition, bond dissociation energies, branching chain reactions.
- vii) **The collision theory:** Dynamics of bimolecular collisions and rate and rate constant of bimolecular reaction, factors determining effectiveness of collisions, Termolecular reactions, unimolecular reactions. Relation between cross section and rate coefficients.
- viii) **Potential Energy Surfaces:** Long range, empirical intermolecular and molecular binding potentials, Internal coordinates and normal modes of vibration, Potential energy surfaces, ab-initio calculation of potential energy surface, experimental

determination of potential energy surfaces, Details of the reaction path, potential energy surface for electronically excited molecule. Molecular beam scattering, State resolved spectroscopic technique, molecular dynamics of $H_2 + H$ reaction, state-to-state kinetics of $F + H_2$ reaction.

- ix) **Transition State Theory (TST):** Motion on the potential energy surface, Basic postulates and derivation of TST, dynamical derivation of TST, Quantum mechanical effects on TST, Thermodynamic formulation of TST, Application of TST, Micro-cannonical TST, Variational TST, Experimental observation of TST.

Texts/References

1. K.A. Connors, Chemical Kinetics : A Study of Reaction Rates in Solution, V.C.H. Publications 1990.
2. J.I. Steinfeld, J.S. Francisco and W.L. Hase, Chemical Kinetics and Dynamics, Prentice Hall 1989.
3. Paul L. Houston, Chemical Kinetics and reaction dynamics.
4. K.J.Laidler, Chemical Kinetics, 3rd ed. Harper and Row, 1987.
5. R.D.Levine and R.B.Bernstein, Molecular Reaction Dynamics and Chemical Reactivity, Oxford University Press, 1987.
6. J.W. Moore and R.G. Pearson, Kinetics and Mechanisms, John Wiley and Sons, 1981.
7. A. A. Forst and R. G. Pearson, Kinetics and Mechanism, Wiley International Edition.
8. Sanjay K. Upadhyay, Chemical kinetics and Reaction Dynamics, Springer, 2006

CB402: Chemistry of Organic Molecules –I

(45 +15 = 60 hrs.)

A. Chemistry of aliphatic compounds: preparation, structure, properties and reactions.

- i) Hydrocarbons: alkanes, alkenes, alkynes. Preparation, Structures and Reactions – substitution, addition and halogenation reactions. Electrophilic addition: rearrangements. Free radical and polar mechanisms. Markownikoff's rule, the peroxide effect, Lemieux reagent, Grignard reagent, Wurtz reaction, Ozonides/Ozonolysis. Stereoselective and Stereospecific reactions. (5 hrs.)
- ii) Monohydric and polyhydric alcohols and ethers (3hrs.)
- iii) Carbonyl compounds – Oxidation, reduction reactions. Meerwin-Pondroff-Verley reduction, Clemenson reduction, Wolf-Kishner reduction, Schmidt reaction, Aldol condensation, Claisen condensation, Claisen-Schmidt reaction, Cannizaro reaction, Tischenko reaction, haloform reaction, Baeyer-Villiger oxidation, Polymer of acetaldehyde, Chloral (5 h).
- iv) Carboxylic acids and derivatives (4hrs.)
- v) Polycarbonyl compounds. Compounds with conjugated double bonds – dienes and enones, α,β -unsaturated compounds – tautomerism. Unsaturated alcohols, ethers, and carbonyl compounds. (5hrs).
- vi) Nitrogen, sulphur, phosphorous, silicon and boron compounds. Aliphatic diazocompounds. (4hrs.)

B. Chemistry of aromatic compounds – preparation, structure, properties and reactions.

- i) Hydrocarbons: monocyclic, polycyclic and condensed systems. Reactivity and orientation. Electrophilic substitution reactions- general methods of preparation of

- benzene homologues, Hammett and Taft equation, Friedel-Crafts reaction. Polynuclear hydrocarbons and their derivatives.
- ii) Halogen, nitro, nitroso, amino compounds. Diazonium salts and their related compounds.
 - iii) Aromatic alcohols, Phenols, ethers, aldehydes, ketones, quinones carboxylic and sulfonic acids.

Text / References:

1. I. L. Finar, Organic Chemistry, Vol. 1 & 2, ELBS.
2. R. T. Morrison and R. N. Boyd, Organic Chemistry, Prentice Hall of India.
3. J. McMurry, Organic Chemistry, Asian Books Pvt. Ptd.
4. L. G. Wade, Organic Chemistry, Pearson Education
5. G. Solomons and C. Fryhle, Organic Chemistry, John Wiley & Sons (Asia) Pte Ltd.
6. M.J.Sienko and R.A.Plane, Chemical Principles and Applications, McGraw Hill, 1980.
7. D.D.Ebbing, General Chemistry, Houghton Mifflin Co., 1984.
8. T.W.G. Solomons, Fundamentals of Organic Chemistry, 5th Ed., John Wiley, 1992.
9. J. March, Advanced Organic Chemistry, 3rd Edn. McGraw Hill, 1991.
10. S.H.Pine, Organic Chemistry, 5th Edn., McGraw Hill, 1987.
11. F.J. Carey and R.J. Sundburg, Advanced Organic Chemistry, Part A and Part B, 2nd Edn. Plenum Press, 1983.

PCB402: Atomic and Molecular Spectroscopy (45 + 15 hrs.)

A. Atomic Spectroscopy (45 + 15 =60 hrs.)

1. The Effect of Radiation on Atoms and Molecules. Transition moment - selection rules for electric dipole, magnetic dipole, electric quadrupole transitions. Width and intensity of spectral transitions. Subdivisions of Spectroscopy.
2. Atomic States, Shells, and Configurations, Hydrogen and Hydrogen-like Ions, Alkalis and Alkali-like Spectra, Helium and Helium-like Ions; *LS* Coupling, Hierarchy of Atomic Structure in *LS* Coupling, Allowed Terms of Levels for Equivalent Electrons, *LS* Coupling, *jj* Coupling.
3. Notations for Different Coupling Schemes: *LS* Coupling (Russell-Saunders Coupling), *jj* Coupling of Equivalent Electrons, *J1 j* or *J1 J2* Coupling, *J1 l* or *J1 L2* Coupling (*J1 K* Coupling), *LSI* Coupling (*LK* Coupling), Coupling Schemes and Term Symbols.
4. Eigenvector Composition of Levels, Ground Levels and Ionization Energies for the Neutral Atoms, Zeeman Effect, Term Series, Quantum Defects, and Spectral-line Series.
5. Sequences: Isoelectronic Sequence, Isoionic, Isonuclear, and Homologous Sequences.
6. Spectral Wavelength Ranges, Dispersion of Air, Wavelength (Frequency) Standards.
7. Spectral Lines: Selection Rules, Intensities, Transition Probabilities, Values, and Line Strengths (Emission Intensities (Transition Probabilities), Absorption *f* values, Line Strengths, Relationships between *A*, *f*, and *S*, Relationships between Line and Multiplet Values, Relative Strengths for Lines of Multiplets in *LS* Coupling)
8. Atomic Lifetimes.

9. Regularities and Scaling: Transitions in Hydrogenic (One-Electron) Species, Systematic Trends and Regularities in Atoms and Ions with Two or More Electrons.
10. Spectral Line Shapes, Widths, and Shifts: Doppler Broadening, Pressure Broadening.
11. Spectral Continuum Radiation, Hydrogenic Species, Many-Electron Systems.
12. Atomic Spectroscopy as a tool for elemental analysis: atomic absorption spectroscopy, atomic fluorescence, Flame photometry, Plasma emission and interfaced ICP-MS. Photoelectron spectroscopy.

Text / References:

1. G. W. F. Darke (ed.), Atomic, Molecular and Optical Physics, AIP Press, Woodbury, NY, 1996).
2. J. W. Robinson, Atomic Spectroscopy.
3. H. E. White, Introduction to Atomic Spectra, McGrawHill Int. Book Company.

B. Molecular Spectroscopy

- i) Born-Oppenheimer approximation - rotational, vibrational and electronic energy levels of homonuclear and heteronuclear diatomic and polyatomic molecules.
- ii) Microwave Spectroscopy: Rotational of molecules and rotational spectroscopy of rigid diatomic molecules, Effect of isotopic substitution, The non-rigid rotator and rotational spectra. Rotational spectra of polyatomic molecules – linear, symmetric top and asymmetric top. Techniques and instrumentation.
- iii) Infrared spectroscopy: energy levels of vibrating diatomic molecule, simple harmonic oscillator and anharmonic oscillator, diatomic vibrating rotator, vibration-rotation spectra of CO. Breakdown of B-O approximation – interaction of rotations and vibrations. Vibrations of polyatomic molecules – Fundamental vibrations and their symmetry, overtone and combination frequencies, influence of rotation on the spectra of polyatomic molecules – linear and symmetric top molecules. Influence of nuclear spin. Group frequencies and analysis of spectra, Techniques and instrumentation, FTIR spectroscopy.
- iv) Raman Spectroscopy: Classical and quantum theories of Raman effect and molecular polarizability. Pure rotational Raman spectra, Vibrational Raman spectra, Polarization of light and the Raman effect, Structure determination from Raman and infrared spectroscopy, Techniques and Instrumentation, Near IR FT Raman spectroscopy. Resonance Raman and electronic Raman transition and applications.
- v) Electronic spectroscopy – Electronic structure and spectra of diatomic and polyatomic molecules. Techniques and instrumentation. Molecular photoelectron spectroscopy.
- vi) Electron spin resonance spectroscopy - spin and spectra - relaxation processes - origin of g-shifts and hyperfine coupling - Tensor quantities - Experimental determination of g, A and D tensors - their interpretation - several examples.
- vii) NMR spectroscopy - Spin - origin of chemical shifts and spin-spin coupling - paramagnetic shifts and their applications - Introduction to relaxation processes in solution.
- viii) Mossbauer spectroscopy - Origin of isomer shifts, G.S. and h.f.s. - applications to structures, phase transitions and material science.

Text/ Reference

1. G. M. Barrow, Molecular spectroscopy
2. C.N. Banwell and E. M. McCash, Fundamentals of Molecular spectroscopy, Tata McGraw Hill Pub. Co. New delhi
3. J. D. Graybeal, Molecular Spectroscopy, McGraw Hill International Book Co. N.Y.

**Third Year
Semester V**

Subject Code	Subject	Contact hrs/per week (Theory +tutorials)	Credits
C501	Quantum Chemistry & Group Theory	3 + 1	4
C502	Chemistry of Inorganic Molecules II	3 +1	4
CB503	Analytical Chemistry	3 + 1	4
G501	Numerical methods	3 + 1	4
G502	Earth Sciences	2 + 1	3
		Contact hrs/per week Lab	Credits
CL501	Chemistry Laboratory	6	6

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C 501: Quantum Chemistry & Group Theory

(45 + 15 = 60 hrs.)

A. Quantum Chemistry:

(35 hrs.)

- a. Foundations of wave mechanics- black body radiation, photons and particles, the Compton effect, particle diffraction, Fourier transforms, superposition of plane waves, wave packets and Einstein-de Broglie relation.
- b. wave function for a free particle, the Schrodinger equation, physical interpretation of the Scrodinger equation wave function, expectation of a dynamical quantity, Wavepackets and the uncertainty principle, WKB approximation and the Bohr-Sommerfeld quantum conditions.
- c. Operator concept in quantum chemistry.
- d. Solution of Schrodinger's equation in some simple systems: one and three dimensional boxes, electron in a ring, rigid rotator, concept of tunnelling, one dimensional harmonic oscillator, hydrogen-like atoms, shapes of atomic orbitals.
- e. Approximate methods of quantum chemistry: variational principle; Huckel Theory; Time-independent perturbation theory: Many electron atoms: Orbital approximation, Slater determinant; Hartree-Fock self-consistent field theory; Slater type orbitals. Concept of LCAO and introduction to ab-initio and semi-empirical molecular orbital calculations of molecules. Extended systems: From bonds to bands. Angular momentum of many-particle systems. Spin orbital interaction; LS and JJ coupling. Spectroscopic term symbols for atoms. Molecules and Chemical bonding: Born-Oppenheimer approximation, MO and VB theories illustrated with H₂-molecule; Spectroscopic term symbols for diatomics; Directed valence & hybridization in simple polyatomic molecules. An elementary treatment of scattering theory.

Text Books:

1. Ira N. Levine, Quantum Chemistry Prentice Hall India.
2. John L. Powell and Bernd Crasemann, Quantum Mechanics, Oxford & IBH Publishing.
3. A. K. Chandra, Introductory Quantum Chemistry, Tata McGraw-Hill Publishing Comp. Ltd.
4. David B. Beard, Quantum Mechanics, Allyn & Bacon, Inc, Boston.

B. Group Theory. (25 hrs.)

1. Symmetry Elements and Operations, Pure Rotations (C_n Rotations), Improper Rotations, Rotation-Reflection (S_n) & Rotation-Inversion (\bar{n}) Axes.
2. Point Groups: Low Symmetry Point Groups (C_1, C_i, C_s), Simple Axial Point groups ($C_n, S_{4n}, C_{nv}, C_{nh}$), Dihedral Groups (D_n, D_{nd}, D_{nh}), Platonic Solids & the "Cubic" Groups (T_d, O_h, I_h), Derived High Symmetry Groups (T, T_h, O, I), The "Infinite Groups" ($C_{\infty v}$ and $D_{\infty h}$), Points Groups & Chirality, Point Groups & Dipole Moment.
3. Multiplication Tables (i.e., operation 1 followed by operation 2) for point groups. Similarity Transforms, Classes of Symmetry Elements. Naming Representations (Mulliken Symbols), Subgroups and Supergroups., Non Commutative Operations.
4. Representations of Groups., Irreducible Representations., Character Tables. Their derivations and use of their contents. Matrix Representation of Symmetry Operations. The "Full Form" of the Character Table.

Text / References:

F. A. Cotton, "Chemical Applications of Group Theory", 3rd Edition, John Wiley (1990).

C502: Chemistry of Inorganic Molecules II: (45 + 15 = 60 hrs.)

C. Coordination chemistry: 30 hrs.

- a. Coordination compounds, Werners's theory, effective atomic number, coordination number, shapes of d-orbitals and bonding in transition metal complexes, stability of complexes, the chelates and macrocyclic effects, types of classification of ligands, second sphere of coordination, π -complexes, π -acid ligands, multiple bonds from ligands to metals.
- b. Crystal Field theory – crystal field splitting and elementary treatment of the electronic spectra, Jahn-Teller distortion of octahedral complexes, square planar complexes, tetrahedral complexes, magnetic properties of 3d compounds (6 h).
- c. MO theory – Nomenclature of coordination compounds, d-orbital splitting in various fields - Spectroscopic states - Tanabe-Sugano and Orgel diagrams - Derivation of Ligand field parameters (Dq, B) from electronic spectra - Magnetic moments - Orbital contribution, spin-orbit coupling and covalency - Molecular orbitals and energy level diagrams for common symmetries.
- d. Bonding involving-donor ligands - Back-bonding - f-orbital splitting - Spectral and magnetic properties of f-block elements.
- f. Reaction mechanisms: Substitution reactions - Dissociative and associative interchange - trans-effect - Linear free energy relations. Rearrangements - Berry pseudo rotation, Electron transfer reactions. Photo-dissociation, -substitution and redox reactions, Fluxional molecules.

B. Chemistry of d-block elements (30 hrs.)

- a) **General introduction to transition elements** – Electronic structure, Metallic character, variable oxidation state, complexes, magnetic and catalytic properties.
- b) **Elements of the first transition series:** Occurrence, separation, extraction and chemistry of the scandium group (IIIB), titanium Group (IVB), vanadium group (VB), chromium group (VIB), Manganese group (VIIB), Iron group (VIIIB(8)), Nickel group (VIII(9)) and Copper group (VIIIB(10)).

Texts/References:

1. F.A. Cotton, G. Wilkinson, C.A. Murillo and M. Bochmann, *Advanced Inorganic Chemistry*, Wiley Eastern, John Wiley, 6th Ed., 1999.
2. J.E. Huheey, E. Keiter and R. Keiter, *Inorganic Chemistry*, 4th Ed., Harper Collins College Publisher, 1993.
3. D.Banerjea, *Inorganic Chemistry Principles*, Books Syndicate Pvt. Ltd., 2000.
4. N.N. Greenwood and E.A. Earnshaw, *Chemistry of Elements*, Pergamon Press, 1989.
5. J.J. Kratz, G.T. Seaborg and L.R. Morss; *The Chemistry of Actinide Elements*, 2nd Edition, Vol. 1&2, Chapman & Hall, New York (1986).
6. J.C. Bailar, H.J. Emelius, R. Nyholm and A.F. Trotman-Dickenson; *Comprehensive Inorganic Chemistry*, Vol. 5, Pergamon Press, Oxford (1973).
7. A.J. Freeman and C. Keller (Eds.); *Handbook of Chemistry and Physics of the Actinides*, Vol. 1-6, North Holland Publishers, Amsterdam (1986).
8. G.R. Choppin and M.K. Khankhasayev; *Chemical Separation Technologies and Related Methods of Nuclear Waste Management*, Kluwer Academic Publishers, Netherlands (1999).
9. G.R. Choppin and J. Rydberg; *Nuclear Chemistry, Theory and Application*, Pergamon Press, Great Britain (1980).

CB503: Analytical Chemistry

(60 hrs.)

- 1) **Statistics in chemical analysis:** Methods of sampling and associated errors, Classification of errors, Propagation of errors, treatment of errors, Normal distribution, Tests of Significance and Confidence Limits.
- 2) **Separation techniques:**
 - a. Solvent Extraction Technique: Conventional, Liquid Membranes – Bulk, Supported and Emulsified, Solid Phase Extraction (SPE).
 - b. Ion Exchange : Conventional , Membranes.
 - c. Chromatography: Gas chromatography (GC), High Performance Liquid Chromatography (HPLC), Ion chromatography (IC).
- 3) **Mass Spectrometry:** Mass Analysers – Magnetic, Quadrupole, Time of Flight (TOF), Ion Cyclotron Resonance, Features – Resolution, Dispersion, Abundance, Sensitivity , Detectors – Faraday Cup, Channeltron, Daly, Ion Sources –Thermal Ionisation (TI), Electron Impact, ICP, GD, Laser Ablation (LA-ICP), Secondary Ionisation (SI), Resonance Ionisation (RI), Matrix Assisted Laser Desorption and Ionisation (MALDI), Hyphenated Technique – IC-MS, HPLC-MS, GC-MS.
- 4) **Thermal Methods:** Thermogravimetric Analysis (TGA), Derivative Thermogravimetric Analysis (DTG), Differential Thermal Analysis (DTA), Differential Scanning Calorimetry (DSC), Evolved Gas Analysis (EGA).
- 5) **Electrochemical Methods:** Introduction, Potentiometry , Ion Selective Electrodes (ISE), Voltammetry & Polarography , Cyclic, Pulse and Stripping Voltammetry, Coulometry and Amperometry, AC Electrochemical Techniques, Scanning Electrochemical Microscopy.

Analytical Chemistry II

- a. Absorption and Emission Spectra. Spectroscope, Spectrograph, Spectrometer. Signal-to-noise ratio, resolving power of the spectrometer, Electromagnetic spectrum. Units of Wavelength, Frequency, Wavenumber and Energy,
- b. Detectors- Photomultiplier Tube (PMT), Charge Coupled Device (CCD), Charge Injection Device (CID), Spectrometers – Czerny Turner, Echelle, Sample Introduction Devices – Flame, Electrothermal, Laser Ablation, Direct Sample Insertion Devices, Interferences, detection limits, sensitivity, Absorption Spectrometry – Flame Atomic Absorption Spectrometry, (FAAS), Electrothermal Atomic Absorption Spectrometry (ETAAS), Optical Emission Spectrometry (OES) with Inductively Coupled Plasma (ICPOES) ,Glow Discharge (GDOES),Fluorescence Spectrometry – Laser Induced Fluorescence (LIF), Recent advances –Continuum Source (CS-AAS), Single Atom Detection.
- c. Magnetic resonance spectroscopic techniques – NMR and EPR.
- d. X-ray diffraction spectroscopy, Electron microscopy and electron diffraction.
- e. **Nuclear Methods:** Activation Analysis – Neutron Activation Analysis (NAA), Charged Particle Activation Analysis (CPAA), X-ray fluorescence (XRF) spectrometry, Ion Beam Analysis – Backscattering Spectrometry (BS), Particle Induced α -ray Emission (PIGE), Nuclear Reaction Analysis (NRA), Elastic Recoil Detection Analysis (ERDA), Particle Induced X-ray Emission (PIXE).

Text /References

1. Encyclopaedia of Analytical Chemistry: Applications, Theory and Instrumentation, Editor R. A. Meyers, John Wiley & Sons Ltd. (2000).
2. D.A. Skoog, D. M. West, F. J. Holler, S.R. Crouch, Fundamentals of Analytical Chemistry, 8th Edition, Thomson (2004).
3. D.A. Skoog, F. J. Holler, T. A. Niemann, Principles of Instrumental Analysis, 5th Edition, Saunders College Publishing (1998).
4. A.I. Vogel, A text book of Quantitative Analysis, 5th Edition Revised by G. H. Jeffery, J. Bassett, J. Mendham and R. C. Denney, ELBS (1989).
5. A. K. De, S. M. Khopkar and R. A. Chalmers, Solvent Extraction of Metals, Van Nostrand, Reinhold (1970).
6. F. Helfferich, Ion Exchangers, McGraw Hill (1962).
7. L. R. Snyder and J. J. Kirkland, Introduction to Modern Liquid Chromatography, 2nd Edition, Wiley (1979).
8. Ion Exchange and Solvent Extraction : A Series of Advances, Editors J. A. Marinsky and Y. Marcus, Marcel Dekker Inc. (1998).
9. High Performance Liquid Chromatography : Principles and Methods in Biotechnology, Editor E. D. Katz, John Wiley and Sons, Chichester (1996).
10. A. Metcalfe, Atomic Absorption and Emission Spectroscopy, Wiley (1987).
11. Jose A. C. Broekaert, Analytical Atomic Spectrometry with flames and Plasmas, Wiley-VCH (2002).
12. J. Sneddon, Advances in Atomic Spectroscopy, Jai Press (1992).

13. John Roboz, Introduction to Mass Spectrometry: Instrumentation and Techniques, Interscience (1968).
14. Inductively Coupled Plasma Spectrometry and its Application, Editor Steve J. Hill, Sheffield Academic Press (1998).
15. W. W. Wendlandt, Thermal Methods of Analysis, 2nd Edition, Wiley (1974).
16. T. Daniels, Kogan Page, Thermal Analysis (1973).
17. A. J. Bard and L. R. Faulkner, Electrochemical Methods, 2nd Edition, Wiley (2001).
18. S. P. Kruger, Principles of Activation Analysis, Wiley Interscience (1971).
19. L.C. Feldman, J. W. Meyer, Fundamentals of Surface and Thin Film Analysis, North Holland (1986).
20. J. C. Miller and J. N. Miller, Statistics for Analytical Chemistry, 2nd Edition, Wiley (1998).
21. Day and Underwood "Quantitative Analysis" –, 5th edition, *Prentice-Hall* (1986) –

Third Year

Semester VI

Subject Code	Subject	Contact hrs/per week (Theory +tutorials)	Credits
C601	Properties of Matter	3 + 1	4
C602	Chemistry of Organic compounds II	3 + 1	4
C603	Chemistry of Inorganic compounds III	3 +1	4
CB604	Biophysical Chemistry	3 +1	4
G601	IPR	2+1	3
		Contact hrs/per week Lab	Credits
CL601	Chemistry Laboratory	6	6

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C 601: Properties of Matter

(45 + 15 = 60 hrs.)

a. Gaseous State

i). Perfect gases and gas laws, law of partial pressures and partial volumes, Graham's law of effusion, critical state and determination of the critical constants, continuity of state, coefficient of expansion and compressibility. ii). The kinetic theory of gases, pressure and temperature of a gas, derivation of the gas laws from the kinetic theory, The Boltzmann constant, Maxwell's law of distribution of molecular velocities, experimental verification of Maxwell's law. iii). Ideal and real gases, deviations of the real gases from the ideal gas laws, collision diameter, van der Waals equation, reduced equation of state, The Dieterici equation, The Berthelot's equation, The equation of Kammerling-Onnes, Virial Theorem and equation of state, compressibility factors, The heat capacity of gases, The principle of equipartition of energy, gas density and vapour density. iv). Collision number and mean free path, transport properties: viscosity, thermal conductivity and diffusivity of gases.

b. The Liquid State: (i) Intermolecular forces – dipole-dipole London forces, hydrogen bonding. (ii) Vapour pressure, determination of vapour pressure, external and internal pressure, boiling point and vapour pressure. (ii) Surface tension, angle of contact and wetting of surface pressure on a curved surface, rise of liquid in a capillary tube, measurement of surface tension. Surface tension and vapour pressure, surface tension and temperature – Eootvos-Ramsay-Shields relation, Macleod's equation, parachor. (iii) Viscosity, measurement of relative and absolute viscosity, viscosity and temperature, molecular weight from viscosity. (iv) refractive index, specific rotation, molar refraction and chemical constitution, optical activity and specific rotation.

c. The Solid State: Crystalline and amorphous solids, Crystals – Steno's law, Haüy's law, Laws of symmetry. Crystals systems and lattices, Crystals and X-rays, Bragg's method of crystal analysis. Different kinds of crystal structures, methods of crystal analysis, electron diffraction, Isomorphism, Heat capacity of solids, Debye's equation. Liquid crystals, magnetic properties - diamagnetic and paramagnetic materials. Ionic, covalent, metallic and coordinate bonds. (ii) Ionic Bond - characteristics of ionic compounds and crystal structures, radius ratio rules and coordination number, close packing. Classification of ionic structures – AX, AX₂ and AX₃ groups. Lattice Energy, Stoichiometric defects – Schottky and Frenkel. Non-stoichiometric defects – metal excess and metal deficiency. Semiconductors and transistors.

- d. Colloids:** The colloidal system, preparation of colloidal systems, classification. Lyophobic sols - optical and electrical properties, effect of addition of electrolytes and applied electric field. Determination of zeta potential by electrophoresis and electroosmotic methods. Origin of charge and the mechanism of flocculation – stability of sols. Properties of Lyophilic sols – viscosity and protective action. Kinetic properties of sols and Brownian motion. Determination of Avogadro's number from vertical distribution of sol particles and by diffusion method. Macromolecules – viscosity and molecular weight of polymers, osmotic pressure, The Donnan equilibrium. Sedimentation and ultracentrifuge, scattering of light. Protein sols, association colloids and emulsions.
- f. Conductance of solutions and electrochemistry:** Faraday's laws of electrolysis, Electrolytic conduction- Arrhenius theory of electrolytic dissociation, strong and weak electrolytes. Migration of ions – transference numbers, Determination of transference number using Hittorf's rule and moving boundary method. Conductance of solutions – electrolytic conductance, determination of conductance, equivalent conductance and concentration, Kohlrausch's law of independent migration of ions, ionic mobilities, temperature dependence. Hydration of ions, the interionic attraction theory. Applications of conductance measurements – degree of dissociation of weak electrolytes, dissociation constants of weak acids, degree of dissociation of water, basicity of organic acids, determination of solubilities of sparingly soluble salts, conductometric titrations, activities of electrolytic solutions, ionic strength. The Debye-Huckel theory of dilute ionic solutions.

Text/References:

1. P.W. Atkins, Physical Chemistry, Oxford University Press, 7th Edition, 2006.
2. G.M. Barrow, Physical Chemistry, 5th Edition, Tata McGraw-Hill, New Delhi, 1992.
3. D.A. McQuarrie and J.D. Simon, Physical Chemistry - a molecular approach, Viva Books Pvt. Ltd. (1998).
4. D.K. Chakrabarty, Adsorption and catalysis by solids, Wiley Eastern, 1990.
5. F.P. Kane and G.B. Larrabee (Eds.), Characterisation of solid surfaces, Plenum, 1978.
6. A.W. Adamson, Physical Chemistry of Surfaces, 3rd Edn., Wiley Interscience, 1976.
A. Clark, The Theory of Adsorption and Catalysis, Academic Press, 1970.

C 602: Chemistry of Organic molecules – II (45 + 15 = 60 Hrs.)

- a) **Chemistry of Alicyclic compounds** – cycloalkanes and cycloalkenes. Factors affecting stability of conformations, conformation of cycloalkanes. Reaction mechanism in alicyclic compound
Conformation of Cyclic System: Monocyclic compounds and Fused ring and Bridged ring Compound. Topicity and Prostereoisomerism & Racemisation and Methods of Resolution. Dynamic stereochemistry: Conformationally rigid and mobile diastereomers, stereoselectivity. Chemistry of Carbon radical (Single electron transfer mechanism): neighboring group participation; non-classical carbocation; S_N^i mechanism. Rearrangements of Carbocation, Freeradical: Allylic, Pinacol/ Pinacolone, 1,2 rearrangements etc and rearrangement to heteroatoms. Pericyclic reaction and FMO approach.
- b) **Chemistry of Heterocyclic compounds:** containing one heteroatom (Furan, pyrrole, pyridine) and more than one heteroatoms (pyrazole, imidazole, oxazole, thiazole, pyrimidine and pyrazines), their derivatives – preparation, properties and reactions.
- c) **Chemistry of Natural Products:**

- i) Terpenoids : Classification, structure, chemistry and biogenesis of some important mono; sesqui, di, and triterpenes.
- ii) Steroids: Sterols and bile acids, estrogens, androgens, gestagens and adrenocortical hormones. Hormone production. Cardiac glycosides. Steroidal triterpenes; biogenesis of steroids and correlation with terpenoids.
- iii) Alkaloids : Characteristic reactions, general methods of degradation, structure and chemistry of some well-known alkaloids.
- iv) Natural Pigments: anthocyanines, Flavones, flavanones, isoflavones, xanthenes, quinones, pterins, chlorophyll and haemin.
- v) Carbohydrates: Stereochemistry, reaction and conformation of monosaccharides, deoxy and aminosugars, hexonic acid and vitamin C, disaccharides, polysaccharides, inositol; glycosides and other glycosides. Chemistry of vitamins A, B, C and E.

Texts/References

- f. I. L. Finar, Organic Chemistry, Vol. 1 & 2, ELBS.
- g. R. K. Bansal, Heterocyclic Chemistry, Synthesis, Reactions and Mechanisms, Wiley Eastern Ltd., 1990.
- h. J.A.J. Joule and G.F. Smith, Heterocyclic Chemistry, ELBS, 2nd Ed., 1982.
- i. F.G. Riddell, The Conformational Analysis of Heterocyclic Compounds, Academic Press, 1980.
- j. L.A. Paquette, Principles of Modern Heterocyclic Chemistry, W.B. Benjamin, Inc., 1978.
- k. B.M. Acheson, An Introduction to the Chemistry of Heterocyclic Compounds, Interscience, 2nd Ed., 1975.

C603: Chemistry of Inorganic compounds III

- A. Chemistry of the elements of the second and third transition elements:** niobium group (Group IVB), Niobium and Tantalum (Group VB), Molybdenum and tungsten (Group VIB); Technetium and Rhenium (Group VIIB), The Platinum group Metals, Ruthenium and Osmium (Group VIII(8)); Rhodium and Iridium (Group VIII(9)), Palladium and Platinum (Group VIII(10), Silver and gold Group (IB(11))).
- B. Chemistry of f-block elements - The lanthanide and actinide elements.**

Book:

- 1. Advanced Inorganic Chemistry, F. Albert Cotton and G. Wilkinson@1988, John Wiley & Sons.

CB604:Biophysical Chemistry

a) Biomolecules and pharmaceuticals:

Purines and nucleic acids, Haemoglobin, chlorophyll and phtalocyanines, Amino-acids, proteins, RNA and DNA, Drug receptor interactions. Approaches to drug design. Drug metabolism. Analgesics, antidepressants, antipsychotics, antiinflammatory agents, cardiovascular agents, diuretics, antibacterials, antibiotics, antivirals, antimalarials, antiamebics, drugs for neoplastic diseases.

- b) General principles of Biophysical chemistry:** a) Hydrodynamics – Sedimentation equilibrium, and rate, diffusional and Brownian motion, dynamic light scattering. b) Thermodynamics and kinetics – equilibria and reactions involving protons, oxidation/reduction reactions and bioenergetics, differential scanning calorimetry,

isothermal titration calorimetry, other methods of determining thermodynamic properties of biological processes, binding equilibrium, equilibrium dialysis, protein stability and crystallization, hydrogen exchange, surface Plasmon resonance, enzyme kinetics, electrophoresis. Thermodynamic fluctuations and Ergodic hypothesis.

- c) **Understanding biophysical systems using physical chemistry:** signal transduction, membrane potentials, transporters and channels, molecular imaging, photosynthesis and vision.
- d) **Single molecule:** fluorescence microscopy, atomic force microscopy, optical tweezers and traps.

Books:

- 2. **Biophysical Chemistry, Alan Cooper, Royal Soc. Chemistry, 2004, ISBN 0-85404-480-9.**
- 3. **Biophysical Chemistry, James P. Allan, ©2008, Wiley-Blackwell ISBN: 978-1-4051-2436-2.**
- 4. Textbook of Biophysical Chemistry, By ~~U-N-Dash~~, McMillan.

**Fourth Year
Semester VII**

Subject Code	Subject	Contact hrs/per week (Theory +tutorials)	Credits
C701	Photochemistry	3 + 1	4
C702	Nuclear Chemistry	3 +1	4
C703	Organometallics & Bio-inorganic Chemistry	3 +1	4
C704	Physical Organic Chemistry	3 +1	4
E701	Elective I	3 + 1	4
		Contact hrs/per week Lab	Credits
CL701	Chemistry Laboratory	6	6

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C701: Photochemistry

(45 + 15 = 60 hrs.)

A. Basic Principles of photochemistry:

a) Photophysical processes: Deexcitation processes for the excited molecules (fluorescence, phosphorescence, delayed emission, nonradiative relaxation, excimer and exciplex formation, heavy atom effect, etc.). Kinetics of excited state processes and quantum yields of different processes.

b) Properties of the excited state: Acid-base properties, redox potential, geometry, dipole moment, dynamic properties of the excited states.

c) Photoinduced processes: Photo-dissociation, photo-ionization, intramolecular charge and proton transfer processes, intermolecular electron and proton transfer reactions, conformational relaxations, intra and intermolecular energy transfer processes and other important photochemical reactions. Kinetics and mechanism of photochemical reactions.

d) Applications of photochemistry: Photosynthesis, vision, solar energy conversion, atmospheric photochemistry, etc.

e) Studies on ultrafast processes: Nanosecond, picoseconds and femtosecond laser flash photolysis, fluorescence time domain spectroscopy with special emphasis on energy transfer and electron transfer reactions and studies on excited state properties.

B. Organic Photochemistry

Distinctive features of photochemical reactions, methods of preparative photochemistry, Photochemistry of alkenes, alkynes and related compounds – geometrical isomerism, electrocyclic processes, sigmatropic shifts, di- π methane reactions, addition, cycloaddition and oxidative reactions. Photochemistry of aromatic compounds – bond cleavage and hydrogen abstraction reactions, cycloaddition reactions, rearrangements of cyclo-hexenones and cyclo-hexadienones, thiocarbonyl compounds. Photochemistry of other organic compounds – imines, imminium salts, nitriles and nitro compounds, azo and diazo compounds, diazonium salts, sulphur and halogenated compounds, photohalogenation and photonitrosation reactions. Photooxidation of alkanes.

C. Inorganic Photochemistry

Introduction to inorganic photochemistry. Photophysical processes. The electronic absorption spectra of inorganic compounds. Characteristics of the electronically excited states of inorganic compounds. Photoelectrochemistry of excited state redox reactions. Photosensitization. Photochemical reactions; substitution, decomposition and fragmentation, rearrangement, and redox reactions. Selective inorganic photochemistry using laser beams. Inorganic photochemistry in biological processes and their model studies. Ligand field photochemistry of d_n complexes, photochemistry of carbonyl compounds, energy conversion (solar) and photodecomposition of water.

Text/References

1. K.K.Rohatagi-Mukherjee, Fundamentals of Photochemistry, Wiley Eastern, 1978.
2. M.S.Wrighton, Inorganic and Organometallic photochemistry, ACS Pub.,1978.
3. V. Balzani and V. Carasiti, Photochemistry of Co-ordination compounds, Academic Press,1970.
4. J. D. Coyle, Introduction to Organic Photochemistry, ISBN

C702: Nuclear Chemistry (60 hrs.)

- a) **Nuclear Stability:** Concept of nucleus and properties, nuclear mass and binding energy, elemental abundance, radioactive decay laws and equilibria. **Nuclear Models:** Liquid drop model, Shell model, Fermi gas model, collective model, optical model, concept of spin, parity electric and magnetic moments, isomerism.
- b) **Modes of Decay:** α decay, β decay, electron captures, γ de-excitation, internal conversion, artificial radioactivity.
- c) **Nuclear reactions:** Energetics, cross-section, centre of mass system, angular momentum, compound nucleus, statistical model, nuclear fission and fusion, nuclear reactors, Heavy ion induced reactions, Accelerators.
- d) **Applications of radioactivity:** Probing by isotopes, preparation of radioisotopes, Szilard-Chamers' reaction, Concept of tracers, chemical yield, radiochemical purity, Application of radiotracers in Chemical Sciences, uses of nuclear radiations, radioisotopes as a source of electricity.
- e) **Elements of Radiation Chemistry:** Interaction of radiation with matter, radiation dosimetry, radiolysis of water and some aqueous solutions, other radiolytic events.

Text / References:

1. G. Friedlander, J. Kennedy, Nuclear and Radiochemistry (1981) –J. M. Miller and J. W. Macias
2. R. D. Evans, Atomic Nucleus (1955)
3. S. Glasstone, Source book of Atomic Energy (1969)
4. G. T. Seaborg, Man made elements (1963).
5. H. J. Arnikaar, Essentials of Nuclear Chemistry (1982).
6. C. Keller, The Chemistry of Transuranium Elements (1971).
7. J.C. Bailar, H.J. Emelius, R. Nyholm and A.F. Trotman-Dickenson; *Comprehensive Inorganic Chemistry*, Vol. 5, Pergamon Press, Oxford (1973).
8. G.R. Choppin and J. Rydberg; *Nuclear Chemistry, Theory and Application*, Pergamon Press, Great Transuranium elements and Transactinides

C703: Organometallics and Bioinorganic Chemistry (45 + 15 = 60 hrs.)

A. Organometallics

Overview, 18-electron rule, square planar complex. Carbonyl ligand – bonding, binary carbonyl complexes, oxygen-bonded carbonyls, other ligands similar to CO, IR spectrum, main group parallels with binary carbonyl. Pi-ligands – linear and cyclic pi systems, NMR spectra of organometallic complexes. Comparative survey of structure and bonding of metal alkyls and aryls, complexes with π acids, CO and related ligands, complexes with olefins, acetylenes and related unsaturated molecules, catalytic properties of mononuclear compounds, stereochemical non-rigidity in organometallic compounds, boranes, carboranes and metallocarboranes, bimetallic and cluster complexes, structure and applications in catalysis, applications of organometallic compounds in organic synthesis, enantioselective synthesis via organometallic compounds, importance of organometallic compounds in certain biological systems. Other important ligands – complexes containing M – C, M = C, M \equiv C bonds, hydride and dihydrogen complexes, phosphines and related ligands.

Organometallic reactions occurring in metal – ligand substitution, oxidative, addition, reductive, elimination. Organometallic reactions involving modification of ligands – insertion and deinsertion, nucleophilic addition to ligands, nucleophilic abstraction, electrophilic reactions. Homogeneous catalysis and heterogeneous catalysis – use of transition metal complexes, hydroformylation reaction, Walker-Smidt synthesis of acetaldehyde, hydrogenation, Monsanto acetic acid process. Transition metal carbene complexes – structure, preparation and chemistry, metathesis and polymerization reactions. Applications of organometallics to organic synthesis and other applications. Metal cluster compounds - metal-metal bond, carbonyl and non-carbonyl clusters, structure and bonding low dimensional solids, clusters in catalysis.

B. Bioinorganic chemistry - biochemistry of iron - its storage, transport and function, copper and zinc proteins, biological activation of oxygen, bioinorganic chemistry of alkali and alkaline earth metal cations, photosynthesis, nitrogen fixation, toxicity of metals. Chemical make up and essential inorganic elements of organisms. Chemistry aspects of metal complexes. Spectral, biochemical and biological methods used in bioinorganic chemistry. Bioinorganic chemistry of Na^+ , K^+ , Mg^{2+} and Ca^{2+} . Role of metal ions in biology : Proteins and enzymes of V, Mn, Fe, Co, Ni, Cu, Zn and Mo. Structural and functional models. Transport and storage of metal ions. Carcinogenicity of chromium. Selenium in biology.

Text/references

- G.O.Spassard, G.L.Miessler, Organometallic Chemistry, Prentice Hall, 1997.
Robert H. Gable, The Organometallic Chemistry of the Transition Metals, Wiley Interscience (2005).
C.Elsehnbroich and A. Salzer, Organometallic Chemistry, 2nd Ed., Wiley VCH, 1992.
F.A.Cotton, G. Wilkinson, C.A. Murillo and M. Bochmann, Advanced Inorganic Chemistry, 6th Edn., Wiley, 1999.
N.N.Greenwood and A. Earnshaw, Chemistry of the Elements, 1st Edn., Pergamon, 1985.
B.F.G. Johnson, Transition Metal Clusters, Wiley, 1980.
G. Wilkinson, F.G.A. Stone and E. Abel, Comprehensive Organometallic chemistry, Pergamon, 1980.

S.J.Lippard & J.M.Berg, Principles of bioinorganic chemistry, University Science Books, Mill Valley, 1994.

I. Bertini, H.B.Gray, S.J.Lippard and J.S.Valentime, Bioinorganic Chemistry, Univ. Sci. Books, Mill Valley, 1994.

James A.Cowan, Inorganic Biochemistry, VCH Publishers, 1993.

Jan. Reedijk, Marcel Dekker,Inc.(Ed.), Bioorganic Catalysis, 1993.

R.W.Hay, Bioinorganic Chemistry, Ellis Hollwood,Ltd.1984.

'Inorganic Chemistry - Principles of Structure and Reactivity', J.E. Huheey; Harper & Row, 1988.

G.L.Geoffrey and M.S. Wrighton, Organometallic Photochemistry, Academic Press, 1979.

C 704: Physical organic chemistry

**Fourth Year
Semester VIII**

Subject Code	Subject	Contact hrs/per week (Theory +tutorials)	Credits
C801	Chemistry of Materials	3 + 1	4
C802	Macro and Supra-molecular chemistry	3 +1	4
E801	Elective I	3 + 1	4
E802	Elective II	3 + 1	4
		Contact hrs/per week Lab	Credits
CL801	Chemistry Laboratory	3	3
CR801	Project		6

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C801: Chemistry of Materials

(60 hrs.)

A. Basic Aspects of the Solid State

Solid State Structure: Primitive lattice vectors - reciprocal lattice - crystal systems and desymmetrization schemes. Bravais lattices; crystallographic point groups and space groups - organic and inorganic crystal structure motifs - polytypes and polymorphs.

Defects and Non-stoichiometry: Intrinsic and extrinsic defects - point, line and plane defects; vacancies, Schottky defects, Frenkel defects - Charge compensation in defective solids - non-stoichiometry, thermodynamic aspects and structural aspects.

Thermal Properties: Free electron theory, electrical conductivity, Hall effect - band theory, band gap, metals and semiconductors - intrinsic and extrinsic semiconductors, hopping semiconductors - semiconductor/metal transition - p-n junctions - superconduction, Meissner effects, type I and II superconductors, isotope effect, basic concepts of BCS theory, manifestations of the energy gap, Josephson devices. Magnetic Properties: Classification of magnetic materials - Langevin diamagnetism - Quantum theory of paramagnetism - cooperative phenomena - magnetic domains and hysteresis - magnetism and dimensionality.

Optical Properties: Optical reflectance - excitons - Raman scattering in crystals - photoconduction - color centers - lasers - photovoltaic effect.

Synthesis of Materials: Phase diagrams - preparation of pure materials, mass transport, nucleation and crystal growth - preparative techniques, zone refining, chemical transport, etc.

Multiphase materials: Ferrous alloys, Fe-C phase transformations in ferrous alloys, stainless steels - non-ferrous alloys - properties of ferrous and non-ferrous alloys and their applications.

Nanocrystalline phase - preparation procedures - special properties - applications.

Thin Films, Langmuir-Blodgett Films: Preparation techniques, evaporation/sputtering, chemical processes, MOCVD, sol-gel etc. - LB film growth techniques - photolithography - properties and applications of thin films, LB films.

Liquids Crystals: Mesomorphic behavior - thermotropic and lyotropic phases – description of ordering in liquid crystals, the director field and order parameters - nematic and smectic mesophases, smectic -nematic transition and clearing temperature - homeotropic, planar and twisted nematics - chiral nematics - smectic A and smectic C phases - cholesteric-nematic transition - optical properties of liquid crystals - effect of external field.

Ionic Conductors: Types of ionic conductors - Mechanism of ionic conduction; interstitial jumps (Frenkel), vacancy mechanism, diffusion - superionic conductors, phase transitions and mechanism of conduction in superionic conductors - examples and applications of ionic conductors.

High T_c Materials: Defect perovskites - high T_c superconductivity in cuprates – preparation and characterization of 1-2-3 and 2-1-4 materials - normal state properties, anisotropy, temperature dependence of electrical resistance, optical phonon modes – superconducting state, heat capacity, coherence length, elastic constants, positron lifetimes, microwave absorption - pairing and multigap structure in high T_c materials - applications of high T_c materials.

Materials for Solid State Devices: Rectifiers, transistors, capacitors - IV-V compounds - low-dimensional quantum structures, optical properties.

Organic Solids, Fullerenes, Molecular Devices: Conducting organics – organic superconductors - magnetism in organic materials.

Fullerenes - doped fullerenes as superconductors

Molecular rectifiers and transistors - artificial photosynthetic devices - optical storage memory and switches - sensors.

Nonlinear Optical Materials: Nonlinear optical effects, second and third order - molecular

hyperpolarisability and second order electric susceptibility - materials for second and third harmonic generation.

Text / References:

1. H.V. Keer, Principles of the Solid State, Wiley Eastern (1993).
2. N.W. Ashcroft, N.W. Mermin, Solid State Physics, Saunders College, Philadelphia (1976).
3. W.D. Callister, Material Science and Engineering. An Introduction, Wiley, New York (1985).

C 802: Macro and Supramolecular Chemistry

(60 hrs.)

A. Polymer Chemistry

1. Polymerization reactions, mechanism and kinetics – cationic, anionic and radical polymerization. Template, emulsion and electrochemical polymerization, Condensation, ring opening, step growth and radiation polymerization reactions. Coordination complex polymerization, Naturally occurring polymers, Biological polymers, inorganic polymers. Polymerization of cyclic organic compounds. Copolymerization and multicomponent polymerization,

2. Thermodynamics and kinetics. Polymerization and depolymerization equilibria - Kinetics of condensation (Step-Growth), Free radical and ionic polymerizations.
3. Physical Characterization: Fabrication and Testing, Relationship between structure and properties - Thermal, flame and chemical resistance - Additives - Electroactive polymers - Biomedical applications. Molecular weight (Mn, Mw) determination - Morphology - Glass transitions and crystallinity - Conformational analysis. Dynamics of dilute polymer solutions and effect of increasing concentration, NMR and neutron scattering studies.
4. Reactions and degradation of polymers, biodegradable polymers. Thermal and oxidative degradation, catalysis by macromolecules, computer applications.

Suggested Reading:

1. H.R. Allcock, F.W. Lampe and James Mark, Contemporary Polymer Chemistry, Prentice Hall, Inc. (1990).
 - l. M.P. Stevens, Polymer Chemistry: An Introduction (2nd Edition) Oxford University Press 1990).
 - m. F.W. Billmeyer, Jr., Textbook of Polymer Science (3rd Edition) Wiley-Inter Science (1984) paperback.
4. A. Ravve, Principles of Polymer Chemistry.

B. Supramolecular Chemistry

- i. Introduction to Supramolecular Chemistry.
- ii. Molecular and Chiral Recognition - Self-Organization, Self-Assembly and Preorganization, molecular and chiral recognition, self-Assembly and self-organization, role of preorganization in the synthesis of topological molecules, template reactions, one-pot' reactions.
- iii. Covalent self-assembly based on preorganization - inclusion complexes, host-guest chemistry, early development of host-guest chemistry. pedersen's works on crown ethers, nomenclature, the structure of inclusion complexes, dynamic character of inclusion complexes, the complexes involving induced fit and without it, endo-hedral fullerene, hemicarcerand and soft rebek's tennis ball-like hosts.
- iv. Mesoscopic Structures as an Intermediate Stage Between Molecules (Micro Scale) on the One Hand and Biological Cells (Macro Scale) on the Other – introduction, medium sized molecular aggregates.
- v. Between Classical Organic Chemistry and Biology Understanding and Mimicking Nature- Introduction, the role of self-organization and self-association in the living nature, modeling processes in living organisms.
- vi. On the Border Between Chemistry and Technology - Nanotechnology and Other Industrial Applications of Supramolecular Systems – introduction, between chemistry and solid state physics - crystal engineering, obtaining crystals with desired properties, nanotechnology and other industrial applications of supramolecular systems, supramolecular catalysis.
- vii. The Most Interesting Macrocyclic Ligands which Are Hosts for Inclusion Complexes- . Crown ethers and coronands, cryptates and cryptands, calixarenes, hemispherands, and spherands, carcerands, hemicarcerands and novel 'molecular flasks' enabling preparation and stabilization of short-lived species, cyclodextrins, and their Complexes, endohedral fullerene complexes,

nanotubes and other fullerene-based supramolecular systems, dendrimers, cyclophanes and steroids forming inclusion complexes, anion binding receptors and receptors with multiple binding Sites.

- viii.** Other Exciting Supramolecular Systems- Making Use of the preorganization phenomenon, topological molecules, multiple hydrogen-bonded systems, organic zeolite, metal directed self-assembly of complex, supramolecular architecture, chains, racks, ladders, grids, macrocycles, cages, nanotubes and self-intertwining strands (helicates).
- ix.** The Prospects of Future Development of Supramolecular Chemistry.

Suggested Reading

1. Recommended Review Articles in the field of supramolecular chemistry.
2. "Supramolecular Chemistry" by F. Vogtle, John Wiley, 1991.
3. "Crystal Engineering. The Design of Organic Solids" by G.R. Desiraju, Elsevier, 1989.
4. Introduction to Supramolecular Chemistry, Dodzuick Helena

**Fifth Year
Semester IX**

Subject Code	Subject	Contact hrs/per week (Theory +tutorials)	Credits
E901	Elective I	3+1	4
E902	Elective II	3+1	4
E903	Elective III	3+1	4
E904	Elective IV	3+1	4
		Contact hrs/per week Lab	Credits
CR900	Project		6

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**Fifth Year
Semester X**

Subject Code	Subject	Contact hrs/week (Theory +tutorials)	Credits
E1001	Elective I	3+1	4
CP1001	Project	-	24

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Elective subjects on Physical Chemistry:

1. Theoretical Organic Chemistry

Structure and Heats of Formation: Classical mechanical approach - Additivity schemes - Relationship between structure and strain - π -electrons within the classical model - Conformational energies - Introduction of - Inter and intramolecular forces. Quantum mechanical approaches - Applications of semi-empirical and ab initio electronic structure methods - Analysis of computational results - Computer experiments.

Reactivity: Substituent effects in reactions - Predictions from theory - Steric and electronic effects - Transition states - A curve crossing model for organic reactions.

Structure - Activity correlations.

Computer Assisted Organic Synthesis.

Suggested Reading:

1. U. Burkert and N.L. Allinger, Molecular Mechanics, ACS Monograph 177, American Chemical Society, Washington DC, 1982.
2. L. Salem and W.L. Jorgensen, Organic Chemists- Book of Orbitals, Academic Press, 1973.
3. T.H. Lowry and K.C. Richardson, Mechanism and Theory in Organic Chemistry, 3rd Edition, Harper and Row, New York, 1987.

2. Advanced Quantum Chemistry

I. Theoretical Treatment of Electron Correlation Effects in Atoms and Molecules

A. Wave Function Theory

1. Review of the principles of quantum mechanics. The Born- Oppenheimer approximation. Many Electron Wave functions.
2. Hartree-Fock approximation. CI. MCSCF.
3. Method of second quantization. MBPT.CCM.
4. Excited states, Greens functions EOM. CCM.
5. Analytical derivatives and properties

B. Density Functional Theory

1. Derivation of the Hohenberg-Kohn theorem
2. Kohn-Sham formulation
3. A review of the performance of the existing local and non-local functionals
4. Treatment of chemical concepts within the density functional theory

II. Computer Experiments using Quantum Chemistry Software Packages

Suggested Reading

N.S. Ostlund and A. Szabo: Modern Quantum Chemistry (McGraw, 1982).

R. McWeeny and B.T.Sutcliffe: Methods of Molecular Quantum Mechanics (Academic, 1976).

R.G. Parr and W. Yang: Density Functional Theory of Atoms and Molecules (Oxford, NY. 1989).

R.M. Dreizler and E.K.U. Gross (Springer-Verlag, 1990).

J. B. Foresman and E. Frisch: Exploring Chemistry with electron structure methods (Gaussian Inc. 1993).

3. Advanced Chemical Dynamics

1. Chemical dynamics : What and why? Pragmatic and puristic approach; Interplay between experiment and theory; State – to state reaction cross section – correlation to thermal rate coefficient
2. Unimolecular reactions : Lindemann theory; Hinshelwood – Lindemann theory, Infra - red multiple photon dissociation / IR laser chemistry – RRKM validation; Laser isotope separation– Atomic and Molecular approaches of LIS
3. Intermolecular potential :Models; potential energy surfaces (PES); attractive versus repulsive; energy consumption and disposal; surprisal analysis; efficacy of vibrational adiabaticity; skewed coordinate representation of PES – mass combination effect.
4. Collision dynamics : Scattering as a probe; differential cross-section; angular deflection function – rainbow and glory impact parameters; quantum mechanical approach to elastic scattering; reaction cross section – reaction probability; opacity function – steric factor; reactive asymmetry – laser pump-probe technique in bulb experiment; angular distribution in reactive collisions – direct reactor versus collision complex; forward, backward and forward – backward scattering; conservation of angular momentum – Newton diagram-lab – to centre of mass transformation.
5. Molecular energy transfer : Microscopic description; relaxation rate equation; hierarchy of ET processes; V-V processes in polyatomics – intra molecular vibrational redistribution process; selectivity of photoexcitation – types of laser induced chemistry; ultrafast reactions; techniques – laser induced fluorescence, femto second transient spectroscopy Molecular beams: unique features; basic beam

scattering apparatus' source – hydrodynamic flow cooling; design considerations; seeded beam – condensation and complex formation; pumping criteria; state selection of reagents.

Reference Books:

1. Molecular reaction dynamics and chemical reactivity - R. D. Levine and R. B. Bernstein, Oxford University Press, New York (1987)
2. Chemical dynamics via molecular beam and laser techniques - R. B. Bernstein, Clarendon Press, Oxford (1982)
3. Chemical applications of molecular beam scattering – M.A.D. Fluendy and K. P. Lawley, Chapman and Hall, London (1973)
4. Molecular beams – N. F. Ramsey, Oxford University Press, New York (1986)).
5. Unimolecular reactions – P. J. Robinson, S.H. Robertson and K. A. Holbrook, Wiley, London (1996)
6. Introduction to molecular dynamics and kinetics – G.D. Billing and K.V. Mikkelsen, Wiley, NY (1996)

4. Computational Chemistry

A brief outline of molecular mechanics, semi-empirical approximations, ab initio methods, basis sets and Z-matrix; Application of these computational methods for prediction of structural and electronic properties of molecules by using standard programs; FMOs in organic chemistry, crystal and ligand field calculations, computation of potential energy surfaces. Conformational analysis by molecular mechanics; Dynamical and structural studies of molecules using molecular dynamics simulations; Monte Carlo simulations of molecules.

Texts/References:

- C. J. Cramer, Essentials of Computational Chemistry: Theories and Models, John Wiley & Sons, 2002.
- David Young, Computational Chemistry: A practical Guide for applying Techniques to Real World Problems, Wiley Interscience, 2001.
- A.R. Leach, Molecular Modelling: Principles and Applications, Pearson Education, 2001.
- J. B. Foresman, A. Frisch, Exploring Chemistry with Electronic Structure Methods. Gaussian Inc., 1996.
- M.P. Allen and D.J. Tildesley, Computer Simulations of Liquids, Oxford, 1987

5. Statistical Mechanics

Ensembles and Averages, equivalence of Ensembles, classical Limit. Monte Carlo and Molecular Dynamics simulations. Distribution functions at equilibrium. Integral equation methods. Perturbation theory. Density functional methods. Molecular fluids. Estimation of thermodynamic functions. Non-equilibrium methods. Linear response theory. Projection operator method. Stochastic processes and Brownian motion. Selected applications to problems in chemical dynamics, relaxation processes and neutron diffraction.

Texts/References

- M.P. Allen and D.J. Tildesley, Computer Simulation in Liquids, Oxford University Press, 1987.

J.P.Hansen and I.R.McDonald, Second Ed., Theory of Liquids, Academic Press,1986.
D.Chandler, Statistical Mechanics, Oxford University Press,1985.
H.L.Friedman, A Course in Statistical Mechanics, Prentice Hall,1983.
L. D. Landau, E. M. Lifshitz and L.P. Pitaevskii, Statistical Physics Parts I and II,
Pergamon Press, 1980

6. Chemical Applications of Group Theory.

1. The Great Orthogonality Theorem Explained.
2. Projections Operators and SALC's (Symmetry Adapted Linear Combinations).
3. Symmetry of Metal-Ligand σ -Bonding in simple $M(X)_n$ ($n = 1-9$) Species.
Rarity of the Symmetrical Cube as a Coordination Environment.
4. Infinite Groups -- Their treatment by Expansion of a Finite Group.
5. Molecular Vibrations Revisited. Force Constants and F and G Matrices.
6. Crystallographic Symmetry. Translational symmetry, screw axes, glide planes and the 230 Space Groups.

Elective subjects on Inorganic Chemistry

1. Environmental Chemistry

Biocycles: C, O₂, N₂, P, S, Co₂, CO₂, etc. Cycles, biodistribution of the elements, chemical separation-

Pollution and its Control

- a. Atmospheric pollution: gaseous air pollution, greenhouse effect and ozone shield, acid-rain particulate air pollution, radiation hazard.
- b. Aquatic pollution: agricultural and pesticidal inorganic and organic pollutants, marine pollution, oil spills and oil pollution.
- c. Industrial pollution: Thermal power, cement, fertilizer, sugar, distillery, drug, paper and pulp and nuclear industry pollution, mining and metallurgy, polymers, etc.

Environmental Analytical Chemistry

Techniques and quantification of pollutants, trace element and radionuclide analysis.

Environmental Toxicology and Detoxification Mechanism

Chemical solutions to environmental problems, better biodegradability, kinetics of decomposition, clean technology, etc.

Suggested Reading

1. Handbook of Environmental Chemistry (Ed. O. Hutzinger) Springer-Verlag, Vol.1-3.
2. Environmental Inorganic Chemistry (Ed. J. Irgolic and A.E. Martell), VCH Publishers.
3. The importance of Chemical speciation- in Environmental Processes (Ed. M. Bernhard, F.E. Brinckman and P.J. Sadler) Springer-Verlag.
4. Environmental Chemistry, Vol. 1 and 2, Specialist Periodical Report, The Chemical Society (London).
5. Environmental Instrumentation (L.J. Fristschen and L.W. Gay) Springer-Verlag.
6. Comprehensive Analytical Chemistry (Ed. G. Svehla) Elsevier, Vol. I_XXVIII

2. Radioisotopes – Production and applications.

Production of Radioisotope

Basic principles of radioisotope production using nuclear reactors and charged particle accelerators. Szilard-Chalmers effect and its utility in radioisotope production.

Concept of radionuclide generators; Growth and decay of activity in a generator;

Different types of ^{99}Mo - $^{99\text{m}}\text{Tc}$ generators; Few other important generator systems such as ^{90}Sr - $^{90\text{Y}}$, ^{188}W - $^{188\text{Re}}$ etc.

Methods of production of some important radioisotopes (such as $^{32/33}\text{P}$, ^{41}Ar , ^{60}Co , ^{79}Kr , ^{82}Br , ^{90}Sr - $^{90\text{Y}}$, ^{99}Mo - $^{99\text{m}}\text{Tc}$, ^{125}I , ^{131}I , ^{137}Cs , ^{153}Sm , ^{166}Ho , ^{177}Lu , $^{186/188}\text{Re}$, ^{192}Ir , and ^{11}C , ^{13}N , ^{15}O , ^{18}F , ^{67}Ga , $^{123/124}\text{I}$, ^{201}Tl etc.).

Calculations of production yields; Bateman's equation and its utility in production yield calculations.

Applications of Radioisotopes in Medicine

Concept of nuclear medicine and radiopharmaceuticals, Classification of radiopharmaceuticals, Characteristics of diagnostic (SPECT and PET) and therapeutic radiopharmaceuticals. Basis of designing radiopharmaceuticals, Methods of radiolabeling, New approaches in radiopharmaceuticals chemistry.

Some important organ-specific diagnostic radiopharmaceuticals (myocardial imaging, brain imaging, renal imaging, tumor and inflammation imaging, receptor-specific imaging agents etc.). PET radiopharmaceuticals – Principle and applications.

Therapeutic radiopharmaceuticals for some specific applications (bone pain palliation, radiation synovectomy, targeted radiotherapy etc.) Concepts of brachytherapy and teletherapy

Quality control of radiopharmaceuticals.

Basic principles of Radiometric assays for in-vitro estimation of hormones, tumour associated antigens etc.

Industrial applications of radiation technology

Fundamental aspects of radiation technology, Ionizing radiation: Sources and Effects, Comparison of different radiation sources for different applications.

Radiation dosimetry

Radiation polymerization, Radiation effects on Polymers,

Radiation Modification of polymers for industrial applications

Radiation sterilization of Medical products

Radiation processing of food

Radiation hygienization of sewage sludge

Radiation processing of flue gases

Application of radioisotopes as tracers in process optimization and trouble shooting in industries.

Isotope tracer applications in hydrology:

Environmental isotopes and artificial radioisotopes in hydrology. Application of environmental isotopes in studying ground water salinity, pollution, recharge etc.;

Artificial radioisotopes in studying dam seepage, effluent dispersion, sediment transport etc.

Reference Books:

1. Manual for Reactor Produced Isotopes. IAEA-TECDOC-1340, IAEA, 1999.
2. Fundamentals of Radiochemistry. D.D. Sood, A.V.R. Reddy, N.Ramamoorthy. 3rd Edition, Indian Association of Nuclear Chemists and Allied Scientists, 2004.

3. Radiopharmaceuticals : Chemistry and Pharmacology Adrian D. Nunn. Marcel Dekker, 1992.
4. Fundamentals of Nuclear Pharmacy. G.B. Saha. 2nd Edition, Springer-Verlag, 1984.
5. Radionuclides in Therapy. R.P. Spencer, R.H. Sievers, A.M. Friedman. CRC Press, Boca Raton, 1987.
6. PET in Oncology : Basics and Clinical Applications, J. Ruhlmann, P. Oehr, H.J. Biersack. Springer-Verlag, 1998.
7. Radioimmunoassay : Principles and Practice, M.R.A. Pillai, S.D. Bhandarkar. 2nd Edition, BARC, 1998.
8. ICRU Report (1980) Radiation Quantities and Units, ICRU Publications, 33
9. Spinks, J.W.T. and Woods R.J. (1990) An introduction to Radiation Chemistry, 3rd edition, John-Wiley, New York-London-Sydney.
10. Pikaev A.K. and Woods R.J. (1994) Applied Radiation Chemistry: Radiation Processing, John-Wiley & Sons Inc., New York, p 341
11. Industrial application of radioisotopes – G. Foldiak
12. Guide Book on Radioisotope Tracers in Industry – Tech. Rep. Series 316, IAEA, Vienna 1990.
13. Environmental Isotopes in Hydrogeology by Ian Clarke and Peter Fritz Lewis Publishers, NY (1997)

3. Advanced techniques in Mass Spectrometry and NMR spectroscopy

Chemical ionization mass spectrometry
 Negative ion mass spectrometry
 Fast atom bombardment mass spectrometry
 Electrospray ionization mass spectrometry
 Matrix assisted laser desorption mass spectrometry
 Tandem mass spectrometry
 Liquid chromatography mass spectrometry
 Nuclear magnetic resonance (NMR) phenomenon and the experimental aspects
 Chemical shift, indirect spin-spin coupling, direct spin-spin coupling
 Relaxation times, nuclear Overhauser effect, polarization transfer
 Two-dimensional NMR, correlation spectroscopy (COSY)
 Nuclear Overhauser effect spectroscopy (NOESY)
 Hetero-nuclear correlation spectroscopy (HETCOR)
 Inverse experiments, hetero-nuclear multiple quantum spectroscopy (HMQC)
 NMR in higher dimensions, NMR of oriented molecules
 Structure and dynamics of bio-molecules
 NMR in the solid state
 Magnetic resonance imaging

Suggested Reading

1. Modern NMR Techniques for Chemistry Research, Ed. Andrew E. Derome.
2. Introduction to Mass Spectrometry, Ed. S.K. Aggarwal and H.C. Jain.

4. Advanced Topics in Inorganic Chemistry

Electron transfer properties of metal complexes. Molecular recognition. Asymmetric catalysis. Phosphorus compounds as ligands. Cluster chemistry. Bio-inorganic reaction mechanisms.

Basic aspects of single crystal diffraction. Molecular metals. Inorganic rings. Transition metal chemistry of macrocycles. Metal ions in medicine. Fluxional molecules.

Text/References

- W.L.Jolly, Modern Inorganic Chemistry, McGraw, Hill Co., 1984.
R.W. Hay, Bioinorganic Chemistry, Wiley, 1984.
M.Day and J.Selbin, Theoretical Inorganic Chemistry, Von. Nostrand, 2nd Ed. 1980.
H.J.Emeleus and J.J. Anderson, Modern Aspects of Inorganic Chemistry, Von. Nostrand, 1962.
J.E.Huheey, Inorganic Chemistry, 4th Ed., Harper Collins College Publisher, 1993.
G.H.Stout and L.H.Jensen, X-ray Structure Determination : A Practical guide, 2nd Ed., John Wiley, 1989.
J.P.Ferraro and J.M.Williams : Introduction to synthetic electrical conductors, Academic Press, 1987.
B.Sarkar (Ed.), Biological Aspects of Metals related Diseases, Raven Press, 1983.
G.A.Melson (Ed.), Coordination Chemistry of Macrocyclic Compounds, Plenum Press, 1979.
D.E.C. Corbridge, The Structural Chemistry of Phosphorus, Elsevier, 1974.
5. Nano- Materials and Soft Condensed Matters

Nano-materials

Introduction: Definition of nano-materials, Difference between bulk and Nano-Materials, Quantum size effect, Evolution of electronic Structure from atoms, clusters, nano-materials to bulk solids, Calculation of surface to volume ratio for different structural arrangements

1.2. Different Class of Nano-Materials : Metal nano-particles, nano-crystals, Clusters and cluster assembled materials (example of C₆₀ solid), Semiconductor nanoparticles, Quantum Well/ wire/Dot Core-Shell nanoparticles Polymers, Organic-inorganic nanocomposite, Nano-structured multilayers Self-Assembly, Bio-Materials (poly-peptide), Nanotubes, nanowires, Nano-rods.

1.3. Synthesis: Chemical precipitation, Sol-Gel method, Ball milling, Physical vapor deposition, Thermal decomposition, Solid state precipitation, Co-sputtering, Silver ion exchange, Ion-implantation, Methods for obtaining monodisperse particles

1.4. Properties: Electronic Properties : (IP, EA, Reactivity, Electronic Structure, DOS etc. Optical Properties : Electron and hole confinement in Semiconductor quantum dots, Band-gap engineering, Optical absorption and photoluminescence, efficiency of optical process, application of nano-particles in non-linear optical devices, Magnetic Property, High density data storage. Thermo-Mechanical Properties .

1.5. Applications: Nano-Catalysis : Electro catalysis, Fuel Cell Materials Bio-medical application, Electronic device application, Molecular Electronics, Spintronics, data storage etc

1.6. Carbon based Nano-Materials: Carbon Clusters, Fullerenes, nano-tubes : Synthesize, Properties and applications.

Soft Condensed Matters:

2.1 Introduction to Soft Matter : Forces, energies, length and time scales in soft matter. Soft matter systems (colloids, surfactants and polymers). Interactions in soft

matter (electrostatic, vander Walls, hydrophilic and hydrophobic interactions, depletion interaction). Soft matter in nature (proteins, polysaccharides, membranes).

2.2 Experimental techniques to investigate structure and dynamics in soft matter : Scattering techniques (Small-angle X-ray scattering (SAXS), Ultra-small-angle-X-ray scattering (USAXS), Small-angle (SANS) and inelastic neutron scattering, Static and Dynamic light scattering (SLS & DLS), NMR, Optical microscopy, digital video microscopy, confocal laser scanning microscopy, Atomic Force Microscopy (AFM), Electron microscopy (TEM & SEM). Optical Tweezers [2 lectures].

2.3 Computer simulations : Molecular dynamics (MD), Monte Carlo (MC), Calculation of pair-correlation function, structure factor, [1 lectures],

2.4 Colloids : Sterically stabilized and Charge stabilized colloids, Colloidal interactions, Synthesis of monodisperse colloidal particles, characterization, Structural ordering, Dynamics, Phase Transitions and applications of colloids [2 lectures].

2.5 Surfactants: Classification, Micellization and critical micelle concentration. Surface tension. Gibbs adsorption equation and surface excess. Phase behavior of surfactants. Cloud point and Kraft temperature. Liquid crystalline phases in surfactants and block copolymers. Langmuir- Blodgett films, Monolayer, Bilayers and Vesicles, [2 lectures]

2.6 Polymer Solutions and Polyelectrolytes : A single ideal chain, mean-squared end to-end distance, radius of gyration. Gaussian chain, Freely jointed chain. Worm-like chain and persistence length. Excluded volume, solvent quality and theta-temperature. Size of a polymer in dilute solutions : osmotic pressure, light scattering and intrinsic viscosity, Polyelectrolytes : Debye-Huckel theory, Donnan equilibrium and Manning condensation. Dynamics of polymeric liquids: Maxwell model. Scaling laws based on Rouse theory, Zimm theory and reptation theory. Polymer Gels: Classes of gels and theory of gelation. [2 lectures].

Reference Books:

1. Nanoparticles and Nanostructured Films: Preparation, Characterization, and Applications, Ed. J.H. Fendler, (Wiley-VCH, New York, 1998)
2. Fundamental properties of Nanostructured Materials, Eds. D. Fiorani (World Scientific, Singapore, 1994)
3. Advanced Catalysts and Nanostructured Materials: Modern Synthetic Methods, Ed. W.R. Moser (Academic, San Diego, 1996)

5. Advanced Coordinate Chemistry

A. Advanced Coordination Chemistry

25 hrs.

Chemistry of Sigma donor and pi-acceptor complexes. Ligand field and molecular orbital theories. Term diagrams in octahedral, tetrahedral and lower symmetries. Electronic dipole selection rules, band intensities, factors influencing band widths. Dichroism studies. Charge transfer spectra. Calculation of ligand field parameters. Magnetic properties of coordination compounds, basic equations of magnetic susceptibility, diamagnetism, paramagnetism, ferromagnetism and antiferromagnetism, temperature independent. paramagnetism and electron delocalisation, effect of zero field splitting. ESR and NMR studies of paramagnetic complexes.

Text/References

1. R.S.Drago, Physical Methods for Chemists, W.B. Saunders Co., 1992.

2. B.N.Figgis, Introduction to Ligand Fields, Wiley Eastern, 1976.
3. A.B.P. Lever, Inorganic Electronic Spectroscopy, Elsevier, 1968.

Elective subjects in Organic Chemistry:

1. Molecular Bio-Organic Chemistry

1. New paradigm in synthesis: Rational synthetic design, convergent and divergent strategies, multi-component and Domino reactions, atom economy, high-throughput synthesis, substrate and reagent-controlled asymmetric synthesis.

2. New paradigm in synthetic approaches: Green strategies, biocatalysis and solvent engineering, microwave and sono-chemistry, non-conventional reaction media (room temperature ionic liquids, super critical fluids, fluorous phase, super-heated steam), template-driven synthesis.

3. New paradigm in functional targets : Design and synthesis of functional molecules/molecular assemblies, non-covalent interactions, electro-magnetic & photoactive organics, organic-inorganic hybrids, organic memory systems for medicinal and separation sciences.

Reference Books

1. Zhu, J. and Bienayme, H.(Eds.) Multi component Reactions. Wiley-VCH Verlag GmbH & Co. 2005.
2. Jung, G. Combinatorial Chemistry: Synthesis, Analysis, Screening, Wiley, 1999.
3. Bannworth, W. and Felder, E. Combinatorial Chemistry: A Practical Approach. Wiley, 2000.
4. Stephenson, G.R. Advanced Asymmetric Synthesis. Chapman & Hall, 1996.
5. Anastas, P.T. and Williamson, T.C. Green Chemistry. Oxford Univ. Press. 1998.
6. Wong, C.H. and Whiteside, G.M. Enzymes in Synthetic Organic Chemistry. Pergamon Press 1994.
7. Gokel, G.W. (Ed) Advances in Supramolecular Chemistry, 2000.
8. Steed, J.W. and Atwood, J.L. Supramolecular Chemistry. Wiley. 2004.