UM-DAE Centre for Excellence in Basic Sciences (CBS)

Course material for 5-year Integrated M. Sc. In Chemistry

First year

Semester I

Subject Code	Subject	Contact hrs/week (Theory +tutorials)	Total no. of hrs.	Credits
M101	Mathematics	2 + 1	30 +15	3
P101	Mechanics & Waves	2 +1	30 + 15	3
C101	Structure of Atoms and Molecules.	2 + 1	35 + 10	3
B101	General Biology	2 + 1	30 + 15	3
G101	Computer basics	2 + 1	30 + 15	3
H 101	Communication Skills	2 + 0	30 + 0	1
PL101	Physics Laboratory	3	45	2
CL101	Chemistry Laboratory	3	45	2
BL101	Biology Laboratory	3	45	2
ML101	Computer Laboratory	3	45	2

C101:Structure of Atoms and Molecules. (35 + 10 = 45 hrs.)

a. ***Atomic structure:*** (i) Charge of electron – Mulliken's experiment. (ii) Atom – scattering of α-particles, Rutherford atoms, Moseley's experiment, atomic number determination. (iii) Atomic spectra, Bohr's theory of atomic structure, Sommerfeld's theory for complex electron spin and magnatic quantum number, Pauli exclusion principle, Hund's rule, electron configuration of elements, Sequence of energy levels and Periodic Table. **(6 +3 = 9 hrs.)**

b. ***Properties of atoms:*** 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. **(6 + 3 = 9 hrs.)**

c. ***Chemical Bonding:*** (i) 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, AX_2 and AX_3 groups. Lattice Energy, Stoichiometric defects – Schottky and Frenkel. Non-stoichiometric defects – metal excess and metal deficiency. Semiconductors and transistors. (iii). 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, 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. (iii) 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. (iv) physical properties and molecular structures – polaizability and dipole moments, melting point, solubility and acid-base properties. **(18 + 9 = 27 hrs.)**

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).

CL101: Chemistry Laboratory (Total 30 hrs.)

Theoretical class: (3hrs.)

Background information, Experiments, Analysis of data, Errors & Statistics, writing reports, observance of laboratory safety.

Inorganic Chemistry Lab - I

A. Basic principles of Chemical Analysis and introduction to common apparatus and basic techniques: (5 hrs.)

(a) **Analytical balance –** essential features, care and use of balance and errors in weighing.

(b) **Burettes and Pipettes –** use of micropipettes.

(c) **Preparation of water for laboratory use** – double and triple distillation, nanopure water.

(d) **General apparatus** – vacuum desicators and dry boxes, heating devices – Bunsen burner and ovens, stirring apparatus – magnetic stirrer, filtration apparatus, distillation apparatus.

(e) Preparation of a standard solution of precisely known concentration of a solute using microbalance and perform titrations to determine the concentration of the solute using both an indicator and a pH probe.

i. Acid-base titration, ii. Redox titration, iii. Precipitation and
iv. complexometric.

B. (a) Inorganic semi-micro qualitative analysis involving 4 radicals: dry and wet tests (22 hrs.)

(b). Volumetric analysis of inorganic ions (15 hrs.).

Text / References

1. D.A. Skoog, D.M. West and F.J. Holler, Analytical Chemistry: An introduction, sixth edition, Saunders College Publisher, 1994.
2. G.H. Jeffery, J.Bassett, J.Mendham and R.C. Denny; Vogel's Text book of Quantitative Chemical Analysis, fifth edition, ELBS, 1991.
3. Vogel: Qualitative Analysis in Inorganic Chemistry.

First year

Semester II

Subject Code	Subject	Contact hrs/week (Theory +tutorials)	Total no. of hrs.	Credits
M201	**Mathematics II**	**2 + 1**	**30 +15**	**3**
P201	**Electricity & Magnetism**	**2 +1**	**30 + 15**	**3**
C201	**Thermodynamics & properties of gases**	**2 + 1**	**35 + 10**	**3**
B201	**Molecular Biology**	**2 + 1**	**30 + 15**	**3**
G201	**Electronics & Instrumentation**	**2 + 1**	**30 + 15**	**3**
H 201	**History of Science**	**2 + 0**	**30 + 0**	**1**
PL201	**Physics Laboratory**	**3**	**45**	**2**
CL201	**Chemistry Laboratory**	**3**	**45**	**2**
BL201	**Biology Laboratory**	**3**	**45**	**2**
GL101	**Electronics Laboratory**	**3**	**45**	**2**

Total no. of hrs.:

C201: Thermodynamics & properties of gases (35 + 10 = 45 hrs.)

a. **Thermodynamics** **(**i) Basic concepts – concept of system, boundary and sorroundings, 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/Cv and C_p – Cv), change of phase and Clapeyron equation, Trouton's rule. (vii) Nernst teat Theorem and third law of thermodynamics, experimental determination of entropy. **(20+ 10 = 30 hrs.)**

b. ***Gaseous State and Kinetic Theory of Gases***: 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. **(10 + 5 = 15 hrs.)**

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. Gaskel , Introduction to to Metallurgical Thermodynamics.
6. K. Denbigh, The principles of Chemical Equilibrium.
7. B. G. Kyle , Chemical & Process Thermodynamics.

CL201: Chemistry Laboratory: (45 hrs.)

A. Physical chemistry Lab –I: (10 hrs.)

Introduction to vacuum techniques and vacuum components

a. To construct vacuum systems from standard components.
b. the uses of different pressure gauges,
c. how to locate leaks in vacuum apparatus,
d. how to use gas cylinders safely,
e. about pumping speed, and how pipes affect it,
f. to use liquid nitrogen and freezing mixtures.
g. Experiments related to thermochemistry (Calorimeter) and gases.

B. Organic Chemistry Lab- I (15 hrs.)

a. Separation and purification of organic compounds (solids and liquids)- crystallization, distillation, solvent extraction, Thin layer chromatography, Column chromatography, gas chromatography.

b. Determination of physical constants (melting points and boiling points) and methods of checking their purity.

C. Inorganic Chemistry Lab –II (20 hrs.)

a. Solvent extraction method – determination of Aluminium as the 8-hydroxyquinoline.

b.Gravimetry – Determination of water of hydration in crystallized barium chloride, estimation of sulphate, chloride, aluminium, manganese, iron, nickel.

c. Use of a ion specific electrode (ISE) to determine the quantity of the ion in a sample.

d. Colorimetry and spectrophotometry – estimation of metal ion e.g. manganese)

Texts/References

1. R.M. Roberts, J.C. Gilbert, L.B. Rodeward and A.S. Wingrove, Modern Experimental Organic Chemistry, Holf-Saunders Intnl.Edn., 4th Edn., 1985.
2. R.L. Shriner, R.C. Fuson and D.Y. Curtin, Systematic Identification of Organic Compounds, a lab. Manual, 6th ed. Wiley, New York.

Second Year

Semester III

Subject Code	Subject	Contact hrs/week (Theory +tutorials)	Total no. of hrs.	Credits
M301	Mathematical Methods	3 + 1	45 +15	4
C301	Properties of Condensed phase	3 +1	45 + 15	4
G301	Statistical Techniques & Applications	2 + 1	30 + 15	3
C302	Chemistry - I	3+ 1	45 + 15	4
H 301	World Literature	2 + 0	30 + 0	1
CL301	Chemistry Laboratory	6	90	6
GL301	Applied Electronics Laboratory	3	45	2

C301: Properties of Condensed phase (45 + 15 = 60 hrs.)

a. ***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. **(9 + 3 =12 hrs.)**

b. ***The Solid State:*** Crystalline and amorphous solids, Crystals – Steno's law, Hauy'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. **(9+ 3 = 12 hrs.)**

c. ***The properties of simple mixtures:*** The thermodynamic description – partial molar quantities. The thermodynamics of mixing, The chemical potential of liquids – ideal solutions and Rault's law, ideal dilute solutions and Henry's law. The properties of solutions – liquid mixtures, colligative properties – lowering of vapour pressure of solutions, elevation of boiling points, depression of freezing point, osmosis and laws of osmotic pressure and thermodynamic derivation of the osmotic pressure law. Deteremination of molecular weights from colligative properties of solutions. Abnormal behaviour of solutions **(6 + 2 = 8hrs.).**

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. **(9+3 hrs. = 12 hrs.)**

e. Conductance of solutions- electrochemistry

Faraday's laws of electrolysis, Electrolytic conduction- Arrhenius theory of electrolytic dissociation, strong and and weak electrolytes. Migration of ions – transference numbers, Determination of transference number using Hittrof'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. **(9+ 3 = 12 hrs)**

f. Adsorption

Gibbs adsorption equation, adsorbent and adsorbate, adsorption isotherm, Langmuir's adsorption isotherm, Types of adsorption,Surface area of adsorbents, surface films on liquids, applications of adsorption. Electrokinetic phenomena – Electro-osmosis, streaming potential, electrophoresis, sedimentation potential. Electrical double layer. Interpretation of electrokinetic phenomena, quantitative formulation for electroosmotic pressure. **(3 + 1 = 4 hrs.)**

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).

C 302: Chemistry –I (45 +15 + 60 hrs.)

A. Organic Chemistry I: (23 + 7 = 30 hrs.)

a) **Introduction**: 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. pπ-dπ bonding – ylides. Delocalization –cross conjugation, resonance. Aromaticity and Huckel's rule – systems of 4n and 4n+2 electrons, antiaromaticity, alternate and non-alternatehydrocarbons. Hyperconjugation. (4 hrs.)

b) **Chemistry of aliphatic compounds**: preparation, structure, properties and reactions.

i) Hydrocarbons: alkanes, alkenes, alkynes. Preparation, Structures and Reactions – substitution, addition and halogenation reactions. Free radical and polar mechanisms. Markownikoff's rule, the peroxide effect, Lemieux reagent, Grignard reagent, Wurtz reaction, Ozonides/Ozonolysis.(5 hrs.)

ii) monohydric and polyhydric alcohols and ethers (3hrs.)

iii) Carbonyl compounds – Oxidation, reduction reactions. Meerwin-Pondroff-Verley reduction, Clemension 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.)

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 Miffin Co., 1984.
8. T.W.G. Solomons, Fundamentals of Organic Chemistry, 5th Ed., John Wiley, 1992.

B: Inorganic Chemistry I: (23 +7 = 30 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) **Descriptive chemistry of main group (s- and p- block) elements:** Hydrogen and rare gases, elements. Occurrence, isolation/extraction and properties. Oxides, hydrides, carbaides, nitrides, halides, oxyhalides, oxiacids,

Text / References:

1. .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.

CL301: Chemistry Laboratory (90 hrs.)

A. **Organic Chemistry Lab – II** **(30 hrs.)**

- **a.** Methods of elemental analysis.
- **b.** Characteristics reactions of functional groups.
- **c.** Identification of unknown organic compounds – chemical and spectral methods.
- **d.** Separation of enatiomers and measurements of optical rotation.
- **e.** Studies of electrophilic / nucleophilic substitution reactions, redox reactions.

B. **Inorganic chemistry Lab – III** **(30 hrs.)**

Complex material analysis of minerals or alloys: Qualitative analysis and quantitative estimation of metal and non-metal ions using conductometry and spectrophotometry. Estimation of iron in iron ore, Estimation of mixture of metal ions by EDTA titrations, Karl Fischer Titration.

C. **Physical Chemistry Lab – II** **(30 hrs.)**

a. Surface tension, viscosity, molecular weight of polymers.
b. Partial molal volumes, partition coefficient, dipole moments, transition temperature determination, colligative properties.

Text / references:

1. G.W.Ewing, "Instrumental Methods in Chemical Analysis", 5th Edition, McGraw-Hill, 1985.
2. D.A.Skoog and J.J.Leary, "Principles of Instrumental Analysis", 4th Editionl, Saunders College Publishing, 1992.
3. B.L. Karger, L.R. Snyder and C. Horvath, An Introduction to Separation Science, John Wiley and Sons, Inc., 1973.
4. J.A. Dean, Chemical Separation Methods, Van Nostrand Reinhold, 1970.
5. D.J. Pasto and C.R. Johnson, Organic Structure Determination, Prentice Hall, 1969.
6. P. C. Rakshit, Physical Chemistry, Science Book Agency, Kolkata.

Second Year

Semester IV

Subject Code	Subject	Contact hrs/week (Theory +tutorials)	Total no. of hrs.	Credits
M401	Mathematical Physics	3 + 1	45 +15	4
C401	Chemical Equilibrium	3 +1	45 + 15	4
C402	Chemistry II	3 + 1	45 + 15	4
G401	Environmental Science	2 + 1	30 + 15	3
H401	History of Indian Mathematics & Astronomy	2 + 0	30 + 0	1
CL401	Chemistry Laboratory	6	90	6
GL401	Applied Electronics Laboratory	3	45	3

C 401: Chemical Equilibrium

a) 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.

b) Law of mass action – mathematical formulation, equilibrium constant from thermodynamic considerations, a few typical reactions in gaseous, liquid and heterogeneous phases, influence of inert gases on the equilibrium state of a gaseous reactions.

c) Thermodynamic criterion for equilibrium: Equilibrium constant and thermodynamic potential change, The reaction isotherm, Standard thermodynamic change, ΔG^0, principle of mobile equilibrium and Le Chatelier's principle.

d) Temperature dependence of equilibrium constant – the reaction isochore, the integration of the Van't Hoff equation, calculation of equilibrium constant of a gaseous reaction, experimental methods for determination of equilibrium constant, equilibrium constant and partition function.

e) Equilibria in heterogeneous systems: Distribution law – Henry's law, solvent extraction, Phase rule and phase diagrams:

   i) one component systems: system H_2O, system CO_2, system sulphur, Enantiotropy, monotropy and dynamic allotropy.

   ii) Two component systems: liquid – liquid phases- system phenol – water, system water – triethylamine, system water – nicotine, influence of foreign substances on critical temperature. Systems with liquid – vapour phases. Completely miscible liquids, ideal solutions, vapour pressure of solutions and rault's law, boiling point composition diagrams, vapour pressure of binary liquid mixtures from thermodynamic considerations (Duem-Margules equation, Konowalof's rule); Partially miscible and immiscible liquids - vapour pressure and distillation diagrams; Solid-liquid phases – thermal analysis and solubility measurement methods; Solid –liquid phases – simple eutectic systems (Sn-Pb, Nathalene-salol, water- KCl), systems separating the component of solid compound with incongruent (Sn –Mg, $FeCl_6$ – H_20) and congruent melting point (NaCl- H2O,

Na_2SO_4 – H_20); binary systems with solid solutions, which are completely miscible and partially miscible (eutectic and peritectic systems); Solid- gas phases – Deliquescence and efflorescence.

iii) Three component systems: simple ternary eutectic systems and system in which one pair is partially miscible.

f) Electromotive force and ionic equilibria: Galvanic cells, reversible and irreversible cells, measurement of EMF of cells, EMF of a cell and free energy change, EMF and equilibrium constant, Different types of single electrodes, Single electrode potentials, Standard electrode potentials, Applications of electrode potentials – determination of valence of an ion, ionic activity, Potentiometric titrations, Liquid junction potential, concentration cells and their applications, Cells in commercial use. Solubility product and solubility. Acids and bases – dissociation constants of weak acid and weak bases, determination of dissociation constants. Ionic product of water, pH and pOH, generalized concept of acids and bases, Determination of pH or H^+ ion concentration (electrolytic and colorimetric methods). Hydrolysis of salt solutions and determination of hydrolysis constants. Buffers and indicators. Polarization and overvoltage. Processes at electrode and metal deposition. **(6 + 2 = 8 hrs.)**

Text / References:

1. L.I. Antrapov, Theoretical Electrochemistry, Mir Publishers, 1972.
2. J.O'M. Bockris and A.K.N. Reddy, Modern Electrochemistry, Vo. 1, Plenum Press,1970.
3. P.W. Atkins, Physical Chemistry, 7th Ed., Oxford University Press, 2006.
4. G.W. Castellan, Physical Chemistry, 3rd Ed. Addison - Wesley/Narosa Publishing House, 1993.
5. D. R. Gaskel , Introduction to Metallurgical Thermodynamics.
6. K. Denbigh, The principles of Chemical Equilibrium.

C 402: Chemistry – II (45 + 15 = 60 Hrs.)

A: Organic Chemistry II: (30 hrs.)

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

i) Hydrocarbons: monocyclic, polycyclic and condensed systems. Electrophilic substitution reactions- general methods of preparation of benzene homologues, Hammett and Taft equation, Friedel-Crafts reaction. Polynuclear hydrocarbons and their derivatives.(8 hrs).

ii) Halogen, nitro, nitroso, amino compounds. Diazonium salts and their related compounds. (5 hrs.)

iii) Aromatic alcohols, Phenols, ethers, aldehydes, ketones, quinones carboxylic and sulfonic acids. (6 hrs.)

b) Alicyclic compounds – cycloalkanes and cycloalkenes (3 hrs.)

c) Heterocyclic compounds: containing one heteroatom (Furan, pyrrole, pyridine) and more than one heteroatoms (pyrazole, imodazole, oxazole, thiazole, pyrimidine and pyrazines), their derivatives – preparation, properties and reactions. (8 hrs.)

Texts/References

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

B: Inorganic Chemistry –II: (30 hrs.)

a) **Descriptive chemistry of *d* block elements:** Transition elements. Occurrence, isolation/extraction and properties. (20 hrs.)

b) **General principles of extraction of metals**. (10 hrs.)

Texts/References:

1. F.A.Cotton and G. Wilkinson, Basic Inorganic Chemistry, Wiley Easter, 1978.
2. M.J.Sienko and R.A. Plane, Chemical Principles and Properties, McGraw Hill, 1975.
3. J.D. Lee, Concise Inorganic Chemistry, Van Nostrand Reinhold, 1977.

CL 401 : Chemistry Laboratory (90 hrs.)

A. Organic Chemistry Lab- III (30 hrs.)

a. Qualitative analysis of organic compounds, Chemical separation binary mixtures and their qualitative analysis.

b. Chemical separation of ternary organic mixtures and characterization of the components – simple one or two step separations involving different techniques.

B: Inorganic Chemistry Lab – IV (30 hrs.)

Complexometric titrations by masking and demasking reactions. Estimations by nephelometry,fluorimetry,simultaneous spectrophotometry, atomic absorption sepectroscopy. Determination of composition of complexes in solution.

C. Physical Chemistry Lab – III (30 hrs.)

Equilibria in solution – phase diagrams. Colligative properties. Electrochemistry – measurements and titrations

Third Year

Semester V

Subject Code	Subject	Contact hrs/week (Theory +tutorials)	Total no. of hrs.	Credits
C501	Chemical Kinetics & Reaction Dynamics	3 + 1	45 +15	4
C502	Inorganic Chemistry III Coordination Chemistry & Chemistry of Lnthanides and actinides	3 +1	45 + 15	4
C503	Organic Chemistry III Stereochemistry & Reaction Mechanisms	3 + 1	45 + 15	4
O501	Numerical methods	3 + 1	30 + 15	3
G501	Earth Sciences	2 + 0	30 + 0	1
CL501	Chemistry Laboratory	6	90	6
CR 500	Project			6

C501: Chemical Kinetics & Reaction Dynamics: (45 + 15 = 60 hrs.)

i) 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) 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. The collision theory – number of bimolecular collisions per unit vol. per second and rate and rate constant of bimolecular reaction, factors determining effectiveness of collisions, Termolecular reactions, unimolecular reactions.

Transition state theory: Potential energy surfaces, partion functions for translation, rotation and vibration, derivation of the rate equation, comparision of collision and transition state theories, transmission coefficient, thermodynamic treatment of reaction rate, free energy of activation and heat of activation and entropy of activation, activated complex theory and RRKM, beams, lasers and mass spectroscopy, state to state reaction dynamics

iii) Comparison of theory with experiment: Simple gas phase reactions, effect of pressure on unimolecular reactions. Reactions in solutionthe influence of solvent on reaction kinetics. kinetics of ionization reaction of neutral molecules, reactions between ions, reactions between ions and neutral molecules, influence of ionic strength, the secondary salt effect.

iv) 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, conscetive second order reactions, reversible reactions, equilibrium from the kinetic view point, complex mechanisms involving equilibria.

v) Catalysis: Homogeneous catalysis in gase 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) Study of rapid reactions: Flow methods, steady state methods, encounter controlled reactions. Quenching of fluorescence, polarography and other diffusion coupled methods, magnetic resonance methods, ion-molecule reactions in the mass spectrometer, relaxation methods, shock methods, a few specific reactions.

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. K.J.Laidler, Chemical Kinetics, 3rd ed. Harper and Row, 1987.
4. R.D.Levine and R.B.Bernstein, Molecular Reaction Dynamics and Chemical Reactivity, Oxford University Press, 1987.
5. J.W. Moore and R.G. Pearson, Kinetics and Mechanisms, John Wiley and Sons, 1981.
6. A. A. Forst and R. G. Pearson, Kinetics and Mechanism, Wiley International Edition.

C502: Inorganic Chemistry III: (45 + 15 = 60 hrs.)

a) Coordination chemistry: (30 hrs.)

i) 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.

ii) Crystal Field theory – crystal filed splitting and elementary treatment of the electronic spectra, Jahn-Teller distortion of octahedral complexes, square planar complexes, tetrahedral complexes, magnetic properties of 3*d* compounds (6 h).

iii) 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.

iv) Bonding involving-donor ligands - Back-bonding - f-orbital splitting - Spectral and magnetic properties of f-block elements.

v) 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) Descriptive chemistry of lanthanides and actinides. (30 hrs.)

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).

C503: Organic Chemistry III (45 + 15 = 60 hrs.)

a) **Stereochemistry:** Optical isomerism, Optical activity and chirality, enantiomers and diasteroisomers, re/si face, optical purity. Geometrical isomerism - Cis-trans isomers, syn and anti isomers. Stereochemistry of alicyclic compounds, biphenyl compounds, Unsaturated dicarboxylic acids, compounds containing elements other than carbon. Conformational analysis and molecular mechanics. Strained molecules. Stereoselective and stereospecific synthesis. (25 hrs.)

b) **Reaction intermediates**: carbocations, carbanions, free radicals, carbenes and nitrenes. Oxidation and reduction of reactions. (5hrs.).

c) Types of reactions, reaction mechanisms and methods of determining them: Substitution, addition and elimination reactions (SN1, SN2, E1 and E2 reactions..). Representative examples and their applications in synthetic organic chemistry. Pericyclic reactions, cycloaddition, cheletropic, electrocyclic, sigmatropicand related reactions, FMO theory. Organic Reagents for reduction, oxidation and other transformations. Name and unnamed reactions- Grignard, Diels-Alder, aldol, Freidel-Crafts, Reformatsky, Cannizzaro, Perkin and related reactions and benzoin condensations etc. (30 h)

Texts/References:

7. R.T. Morrison and R.W. Boyd, Organic Chemistry, 5th Ed., Wiley Eastern, 1992.
8. J. March, Advanced Organic Chemistry, 3rd Edn. McGraw Hill,1991.
9. S.H.Pine, Organic Chemistry, 5th Edn., McGraw Hill, 1987.
10. F.J. Carey and R.J. Sundburg, Advanced Organic Chemistry, Part A and Part B, 2nd Edn. Plenum Press, 1983.

CL 501: Chemistry LAB 90 hrs.

A. Physical Chemistry Lab.

Experiments related to chemical kinetics.

B. Organic Chemistry Lab.

a) Preparation of organic compounds to illustrate the application of synthetically important reactions, purification and characterization.

C. Inorganic Chemistry: Preparation and characterization of coordination comounds.

Third Year

Semester VI

Subject Code	Subject	Contact hrs/week (Theory +tutorials)	Total no. of hrs.	Credits
M601	Mathematical Physics II	3 + 1	45 + 15	4
C601	Quantum Chemistry & Group theory	3 + 1	45 +15	4
C602	Organic Chemistry IV: Chemistry of Natural Products & Biomolecules	3 +1	45 + 15	4
C603	Analytical Chemistry	3 + 1	45 + 15	4
G601	Energy	2 + 1	30 + 15	3
CL601	Chemistry Laboratory	3	60	3

C 601: Quantum Chemistry & Group Theory (45 + 15 = 60 hrs.)

A. **Quantum Chemistry:** **(35 hrs.)**

Classical vs. quantum mechanics, optical spectra, black body radiation, photoelectric effect, Bohr atom. (ii). Foundations of wave mechanics- photons and particles, the Compton effect, particle diffraction, Fourier transforms, superposition of plane waves, wave packets and Einstein-de Broglie relation. (iii). 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 (iv) Operator concept in quantum chemistry. (v) 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. (vi) 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 H_2-molecule; Spectroscopic term symbols for diatomics; Directed valence & hybridization in simple polyatomic molecules. An elementary treatment of scattering theory.

B. Group Theory. **(25 hrs.)**

1. Symmetry Elements and Operations, Pure Rotations (C_nRotations), Improper Rotations, Rotation-Reflection (S_n) & Rotation-Inversion (n-bar) Axes.
2. Point Groups: Low Symmetry Point Groups (C_1 ,C_i , C_s), Simple Axial Point groups (c., S_{4n}, C_{nv}' C_{nh}), Dihedral Groups (D_n, , D_{nd}, D_{nh}), Platonic Solids & the "Cubic" Groups (T_d, 0_h , I_h), Derived High Symmetry Groups (T, T_h , 0, 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).

C602: Organic Chemistry IV: (45 + 15 = 60 hrs.)

A. **Chemistry of Natural Products:** (40 hrs.)

i) Terpenoids : Classification, structure, chemistry and biogenesis of some important mono; sesqui,di, and triter penes.

ii) Steroids: Sterols and bile acids, estrogens, androgens, gestogens 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, xanthones, quinones, pterins, chlorophyll and haemin.

v) Carbohydrates: Stereochemistry, reaction and conformation of monosaccharides, deoxy and aminosugars, hexonic acid and vitamin C, disaccharides, polysaccharides, inositol; gan- gliosides and other glycosides. Chemistry of vitamins A,B,C and E.

B. **Biomolecules and pharmaceuticals**:

i) Purines and nucleic acids
ii) Haemoglobin, chlorophyll and phtahlocyaninnes.
iii) Amino-acids, proteins, RNA and DNA
iv) Drug receptor interactions. Approaches to drug design. Drug metabolism.
v) Analgesics, antidepressants, antipsdychotics, antiinflammatory agents, cardiovascular agents, diuretics, antibacterials, antibiotics, antivirals, antimalarials, antiamoebics, drugs for neoplastic diseases.

Text / References:.

vi) A.Burger, Medicinal Chemistry, 4th Ed., Wiley Interscience, 1981.
vii) R.F. Doerge, Ed., Wilson and Gisveld's Text Book of Organic Medicinal and Pharmaceutical chemistry, 8th Ed., J.B. Lippincott Co., 1982.
viii) D. Lednicer and L.A. Mitscher, The Organic Chemistry of Drug Synthesis, Wiley Interscience, 1977.
ix) O.L.Salerini, Natural and Synthetic Organic Medicinal Compounds, C.V. Mosby Co., 1976.

C603: Analytical Chemistry (60 hrs.)

a) Separation techniques – principles and applications:

1) Solvent Extraction Technique: Conventional, Liquid Membranes – Bulk, Supported and Emulsified, Solid Phase Extraction (SPE).
2) Ion Exchange : Conventional , Membranes.
3) Chromatography: Gas chromatography (GC), High Performance Liquid Chromatography (HPLC), Ion chromatography (IC)

b) **Instrumental methods – principles and applications:**

1) Spectrochemical Methods: 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.
2) 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.
3) Thermal Methods: Thermogravimetric Analysis (TGA), Derivative Thermogravimetric Analysis (DTG), Differential Thermal Analysis (DTA), Differential Scanning Calorimetry (DSC), Evolved Gas Analysis (EGA).
4) Electrochemical Methods: Introduction, Potentiometry , Ion Selective Electrodes (ISE), Voltammetry & Polarography , Cyclic, Pulse and Stripping Voltammetry, Coulometry and Amperometry, AC Electrochemical Techniques, Scanning Electrochemical Microscopy.
5) 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 γ-ray Emission (PIGE), Nuclear Reaction Analysis (NRA), Elastic Recoil Detection Analysis (ERDA), Particle Induced X-ray Emission (PIXE)

C) **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

Text /Rreferences

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) –

CL 601: Chemistry Laboratory (60 hrs.)

A. Analytical Chemistry experiments

Determination of trace impurities in high purity materials by AAS.
Application of Electroanalytical Methods to trace analysis
TGA and DTA study of inorganic compounds.
Mass spectrometry
Characterisation – microscopy, spectroscopy, diffraction..
Properties – conductivity, magnetism, luminescence.

CL 601: Chemistry Lab.

A. Organic chemistry:

Pharmaceutical Chemistry : Synthetic methods for bulk drugs – illustrative computer experiments on drug design principles.

B. **Physical Chemistry:** Computational Chemistry

Fourth Year

Semester VII

Subject Code	Subject	Contact hrs/week (Theory +tutorials)	Total no. of hrs.	Credits
C701	Atomic & Molecular Spectroscopy	3 + 1	45 +15	4
C702	Radioactivity & Nuclear Chemistry	3 +1	45 + 15	4
C703	Biochemistry	3 + 1	45 + 15	4
O701	Radiation Science	3 + 1	45 + 15	4
E701	Elective I	2	30	2
E702	Elective II	2	30	2
OL701	Radiation Laboratory	3	45	3
CL701	Chemistry Laboratory	3	45	3
CR701	Project			6

C701: Atomic & Molecular Spectroscopy (45 + 15 =60 hrs.)

A. Atomic Spectroscopy (25 hrs.)

1. 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, 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), *LS1* 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: (35 hrs.)

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, symmetruic 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 Ranman 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 HillPub. Co.New delhi
3. J. D. Graybeal, Molecular Spectroscopy, McGraw Hill International Book Co. N.Y.

C702: Radioactivity and 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 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. Arnikar, 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: Biochemistry: (45 + 15 = 60 hrs.)

Cell Structure and Function: Structure of prokaryotic and eukaryotic cells, intracellular organelles and their function, comparison of plant and animal cells.

Introduction of biomolecules: Examples of biomolecules, building blocks of biopolymers, types of reactions occurring in cells, structure of ice and liquid water, hydrogen bonding and hydrophobic interactions, buffers and the Henderson-Hasselbalch equation.

Structure of water. Biological relevance of chemical potential. Hydrophobic and hydrophilic interactions in biological systems. Protein-Solvent Interactions - preferential binding, hydration and exclusion. Protein structure, stability, folding, unfolding and their studies with spectroscopic and calorimetric methods. Protein-Ligand Binding. Structure-Function relationships. Equilibria across membranes. Determination, amino acid analysis and the Edman degradation (protein sequencing), Ramachandran plot and the secondary structure of proteins - _ -helix, _ -pleated sheet, _ -bend and collagen triple helix. Tertiary structure and structural motifs – protein folding and domain structure of proteins. Oligomeric proteins. Purification and characterization of proteins, functions of proteins.

Enzymes and catalysis: Substrate specificity of enzymes, requirement of coenzymes, regulation of enzyme activity and allosteric effect, enzyme nomenclature, enzyme kinetics and the Michaelis-Menten equation, various types of enzyme inhibition.

Application of enzymes in chemical synthesis, enzyme models and their applications.

Carbohydrates: Monosaccharides, oligosaccharides and polysaccharides, carbohydrates of glycolipids and glycoproteins, role of sugars in biological recognition, blood group substances.

Lipids and membranes: Common classes of lipids - glycerolipids, phospholipids, sphingolipids and glycolipids. Self-association of lipids - formation of micelles, reverse micelles and membranes, gel and liquid-crystalline phases. Lipid phase polymorphism - bilayer, hexagonal and cubic phases. Liposomes and their properties and applications.

Biological membranes and the fluid mosaic model, current models of biological membranes, membrane proteins and their functions, membrane asymmetry.

Introduction to metabolism: Overview of metabolism, catabolic and anabolic processes, glycolysis, citric acid cycle and oxidative phosphorylation.

Nucleotides and nucleic acids: Ribonucleotides and deoxyribonucleotides, RNA and DNA, base pairing, double helical structure of DNA, forces stabilizing nucleic acid structure, methods used in nucleic acid separation and characterization, supercoiled DNA and topoisomerases, nucleic acid sequencing. Transcription and translation: Messenger RNA, RNA polymerase and protein synthesis.

Control of transcription, protein-DNA interactions. The genetic code, tRNA structure and codon-anticodon interactions. Ribosomes and their structure. Gene cloning and sitedirected mutagenesis.

Text / References:

1. Biochemistry by D. Voet & J. G. Voet, II Edition (1995) John Wiley
2. Principles of Biochemistry by Lehninger, Nelson & Cox, III Edition (1993) CBS publishers, New Delhi.
3. Biochemistry by L. Stryer, IV Edition (1995) W. H. Freeman.
4. Roger B. Gregory, ed., Protein-Solvent Interactions, Marcel Dekker,Inc., 1995.
5. Barry T. Nall and Ken A. Dill, ed., Conformations and Forces in Protein Folding, Americal Association for the Advancement of Science, 1991.

6. Carl Branden and John Tooze, Introduction to Protein Structure, Garland Publishing, Inc., 1991.

7. Jeffries Wyman and Stanley J.Gill, Binding and Linkage : Functional Chemistry of Biological Macromolecules, University Sciences Books, 1990.

8. C.R.Cantor and P.R.Schimmel, Biophysical Chemistry, Part III, W.H.Freeman and Co., 1980.

CL 701: Chemistry Laboratory (45 hrs.)

A. Physical Chemistry:

Experiments related to Atomic and molecular Spectroscopy

1. FTIR spectra of a molecule and identification of spectral bands.
2. Raman spectra a simple molecule.
3. ^{1}NMR spectra of an organic compound and assignment.
4. ESR spectrum of a transition metal complex.
5. Electronic spectra of a transition metal complex (d-d transitions).
6. Infrared spectra of a simple molecule and a transition metal complex.
7. H NMR spectra of an organic compound and of a complex of a non-transition metal.
8. ESR spectrum of a Cu(II) complex
9. Mossbauer spectrum of a Fe compound.
10. d-d transitions.

B. Organic Chemistry

Experiments on Biochemistry

.

C. Inorganic Chemistry:

Experiments on radioactivity and nuclear chemistry, Neutron Activation Analysis of trace constituents in a complex matrix Materials Chemistry

CR 701: Project:

Fourth Year

Semester VIII

Subject Code	Subject	Contact hrs/week (Theory +tutorials)	Total no. of hrs.	Credits
C801	Photochemistry	3 + 1	45 +15	4
C802	Organometallics & Bioinorganic Chemistry	3 +1	45 + 15	4
C803	Inorganic Chemistry IV	3 + 1	45 + 15	4
G801	Biophysics	2 + 1	30+ 15	3
E801	Elective III	2	30	2
E 802	Elective IV	2	30	2
CL801	Chemistry Laboratory	3	45	3
CR801	Project			6

C801: 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 and picosecond 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

Distintive 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. Photoelectochemistry of excicted 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

C 802: Organometallics and Bioinorganic Chemistry (45 + 15 = 60 hrs.)

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. Other important ligands – complexes containing M – C, M= C, M ≡ 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 carbine complexes – structure, preparation and chemistry, metathesis and polymerization reactions. Applications of organometallics to organic sysnthesis and other applications. Metal cluster compounds - metal-metal bond, carbonyl and non-carbonyl clusters, structure and bonding low dimensional solids, clusters in catalysis.

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.

Historical background, factors controlling metal-carbon bond formation, methods of M-C bond formation, comparative survey of structure and bonding of metal alkyls and aryls,complexes with p 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.

Text/references

G.O.Spessard, G.L.Miessler, Organometallic Chemistry, Prentice Hall, 1997.

Robert H. Gabtree, The Organometallic Chemistry of the Transition Metals, Wiley Interscience (2005).

C.Elsehenbroich 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, lst 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 Catlysis, 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 702: Inorganic Chemistry IV (60 hrs.)

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, Elesevier, 1968.

B. Synthesis, properties and characterization of Inorganic Compounds and complexes. (20 hrs.)

Preparative chemistry of compounds and complexes of main group, and transition elements and lanthanides including inorganic chains, rings, cages, clusters, halogen and rare gas compounds. Experimental problems encountered in the synthesis, isolation, purification, characteization and identification of inorganic compounds. Physical methods for characterization, PES, EXAFS, Mossbauer spectroscopy, magnetic susceptibility and cyclic voltammetry. Imporatant properties of the complexes of transition metals, lanthanides and actinides.

Text/References

1. R.S.Drago, Physical Methods for Chemists, Saunders, 1992.
2. R.J.Angelias, Synthesis and Techniques in Inorganic Chemis- try, 2nd Edn., Saunders, 1977.
3. G.Pass and H. Sutchliffe, Practical Inorganic Chemistry: Preparation, Reactions and Instrumental Methods, 2nd Edn., Chapman and Hall, 1974.
4. W.L.Jolly, The Synthesis and Characterisation of Inorganic Compounds, Prentice Hall, 1970.

C. Interfacial Phenomena on metal and semiconductors (15 hrs.)

Adsorption isotherms: Langmuir, BET, Frumkin, Temkin and Freundlich. Adsorption on porous solids. Chemisorption of gases on metals and semiconductors. Kinetics of adsorption processes, heterogeneous catalysis. Catalysis by metals, semiconductors and solid acids. Characterization of solid surface structure and composition using electron microscopy, FEM, XPS, Auger, Mossbauer, SIMS, ISS and LEED.

Text/References

1. D.K.Chakrabarty, Adsorption and catalysis by solids, Wiley Eastern, 1990.
2. F.P.Kane and G.B.Larrabee (Eds.),Characterisation of solid surfaces, Plenum, 1978.
3. A.W.Adamson, Physical Chemistry of Surfaces, 3rd Edn.,Wiley Interscience, 1976.
4. A. Clark, The Theory of Adsorption and Catalysis, Academic Press, 1970.

CL 801: Chemistry Laboratory (45 hrs.)

A. Physical Chemistry:

Experiments related to photochemistry.

B. Inorganic Chemistry

Preparation of selected inorganic metal complexes and their studies by infra red, electronic spectra, Mossbauer, e.s.r. and magnetic susceptibility measurements. Handling of air and moisture sensitive inorganic compounds.

C. Organic & Inorganic Chemistry: Experiments related to organometallics and Bioinorganic and Biochemistry

Fifth Year

Semester IX

Subject Code	Subject	Contact hrs/week (Theory +tutorials)	Total no. of hrs.	Credits
C901	Lasers & Their Applications	3 + 1	45 +15	4
C902	Industrial Chemistry	3 +1	45 + 15	4
C903	Chemistry of Materials	3 + 1	45 + 15	4
G904	Astronomy & Astrophysics	3 + 1	45+ 15	4
E901	Elective V	2	30	2
E902	Elective VI	2	30	2
CL901	Chemistry Laboratory	3	45	3
CR901	Project			6

C901: Lasers and their Applications: (60 hrs.)

A. Introduction to Lasers

1. Rate equation for absorption, induced and spontaneous emission, Einstein's A and B coefficients – Concepts of laser action and population inversion – rate equations for two, three and four level systems.
2. Laser and its sub-systems – Optical amplifier – optical resonator – excited state pump – Properties of laser beams – Spatial and temporal coherence.
3. Different types of passive resonators, modes of a passive resonator – Active resonators – Gain & Threshold condition for lasing actions – laser modes – Gain saturation and mode competition – spatial and velocity hold blowing.
4. Wavelength and Intensity stabilization of lasers – turning of wavelength of lasers – prisms, grating and elations – controlled wavelength turning – Selection of axial modes, Experimental realization of single mode.
5. Generation of short pulses – Q-switching and mode locking
6. Principles of various types of lasers – UV, vis & IR lasers, metal vapour lasers, solid state lasers, Gas lasers, Dye lasers, Semiconductor-diode laser and free electron laser

B. Laser Spectroscopic Techniques:

Important features of lasers useful for spectroscopy – monochromaticity, directionality, high intensity, tunability, short pulses etc. Advantages of lasers for spectroscopy – high sensitivity and selectivity. Short review of spectral line broadening mechanisms.

1. Doppler-limited spectroscopy
   a) High sensitivity methods of Absorption – frequency modulation, intracavity absorption.
   b) Photoacoustic spectroscopy
   c) Resonance ionization spectroscopy combined with mass spectrometry
   d) Optogalvanic spectroscopy
2. Laser Induced Fluorescence
   a) Molecular Spectroscopy by LIF

b) Experimental aspects and advantages of LIF
c) LIF in supersonic molecular beams

3. Laser Raman Spectroscopy
   a) Linear Raman Spectroscopy
   b) Non-linear Raman Spectroscopy – Stimulated Raman scattering
   c) Coherent Anti-Stokes Raman Spectroscopy (CARS)
4. Analytical applications of lasers
   a) Laser induced break down spectroscopy, cavity ring down spectroscopy
   b) Laser Induced Chemical Reactions/ Laser Isotope Separation
   c) Atmospheric measurements with LIDAR

Reference Books:

1. Introduction to lasers and their applications – Donald C. O'shea
2. Introduction to Lasers Physics – K. Shimoda
3. Laser Spectroscopy basic concepts and Instrumentation – W. Demtroder
4. Principles of lasers – O. Svelto and D. C. Hanna
5. Chemical and biochemical applications of lasers-vol I & III, Ed. C.B. Moore, Academic Press, New York (1974)
6. P.W. Milonni and J.H. Eberly, "Lasers", World Scientific, Singapore (1981)

C 902: Industrial Chemistry (60 hrs.)

A. Economic aspects, Pollution prevention and waste minimization, pollution control technology, Applied statistical methods and the chemical industry, Safety consideration in the chemical process industry, managing emergency preparedness.

B. Industrial Gases: carbon dioxide, carbon monoxide, sulphur dioxide, hydrogen, oxygen, nitrogen, rare gases of the atmosphere, coal gas, water gas, producer gas manufacture,

C. liquified petroleum gases, petrochemicals and downstream products related to rubber and polymer, explosives and rocket fuels. Manufacture of cement, glasses, carbon black, abrasives, fertilizers, pulp and paper.

D. Soaps and detergents, perfumes, fertilizers, woods and wood products, synthetic resins and plastics, polymeric materials.

E. Glasses, Ceramics and Composites: Glassy state - glass formers and glass modifiers - applications. Ceramic structures - mechanical properties - clay products - refractories - characterizations, properties and application. Microscopic composites, dispersion-strengthened and particle-reinforced - fiber-reinforced composites - macroscopic composites.

C602: 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 in organic crystal structure motifs - polytypes and polymorphs.

Defects and Non-stoichiometry: Intrinsic and extrinsic defects - point, line and plane defects; vacancies, Schottky defects, Frenker 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 - semi-conductor/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: Mesmorphic behavior - thermotropic and lyotropic phases – description of ordering in liquid crystals, the director field and order parameters - nematic and semectic 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 Tc Materials: Defect pervskites - high Tc 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 Tc materials - applications of high Tc 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).

CL901: Chemistry Lab.

A. Physical chemistry Lab: Experiments related to laser spectroscopy

a) REMPI With TOFMS
b) Laser opto-galvanic spectroscopy
c) LIF spectroscopy

B. Industrial chemistry lab.

Materials Chemistry : Synthesis – polymers, colloids, gels etc.; Characterisation – microscopy, spectroscopy, diffraction..; Properties – conductivity, magnetism, luminescence. Analysis of an alloy sample by EDXRF. Anion analysis by ion selective electrode. Chromatographic separation and measurement of the components in a mixture, Isotopic Analysis by Mass Spectrometry

C. **Material Chemistry**:

Synthesis and Characterization of nanomaterials

CR 901: Project

Fifth Year

Semester X

Subject Code	Subject	Contact hrs/week (Theory +tutorials)	Total no. of hrs.	Credits
C1001	**Project**			**9**

Elective courses:

Physical Chemistry

1. Theoretical Organic Chemistry
2. Advanced Quantum Chemistry
3. Advanced Reaction Dynamics
4. Computational Chemistry.
5. Statistical Mechanics
6. Chemical applications of Group theory
7. Photonics and non-linear optical materials.
8. Physical organic chemistry (solvents and solvent effects on reaction dynamics and mechanism)

Inorganic Chemistry:

1. Environmental Chemistry
2. Radio isotopes and Applications
3. Advanced techniques in mass spectrometry and NMR Spectroscopy
4. Advanced topics in Inorganic Chemistry
5. Nano materials and Soft condensed matters
6. Chemical applications of Group theory
7. Photonics and non-linear optical materials.
8. Physical organic chemistry (solvents and solvent effects on reaction dynamics and mechanism)

Organic Chemistry:

1. Theoretical Organic Chemistry
2. Polymer Chemistry
3. Supramolecular Chemistry
4. Advanced methods in Organic Synthesis.
5. Molecular Bio-Organic Chemistry
6. Chemical applications of Group theory
7. Photonics and non-linear optical materials.
8. Physical organic chemistry (solvents and solvent effects on reaction dynamics and mechanism)

Elective subjects on Physical Chemistry:

1. **Theoretical Organic Chemistry**

   Structure and Heats of Formation: Classical mechanical approach - Additivity schemes - Relationship between structure and strain - -electrons within the classical modelπConformational energies - Introduction of - Inter and intramolecular forces.
   Quantum mechanical approaches - Applications of semi-empirical and ab intio electronic structure methods - Analysis of computatioinal 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 Editiion, Harper and Row, New York, 1987.

2. **Advanced Quantum Chemistry**

   I. Theoretical Treatment of Electron Correlatiion 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 thoery

   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 Dyamics 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 o-Bonding in simple $M(X_{nn}$ (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, O_2, N_2, P, S, Co_2, CO_2, etc. Cycles, biodistribution of the elements, chemical -sepration-.

Pollution and its Control

a. Atmospheric pollution: gaseous air pollution, greenhouse effect and ozone shield, acid-rain particulate air pollutiion, radiation hazard.

b. Aquatic pollution: agricultural and pesticidal inorganic and organic pollutants, marine pollution, oil spills and oil pollutiion.

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-^{99m}Tc generators; Few other important generator systems such as ^{90}Sr-^{90}Y, ^{188}W-^{188}Re etc.

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

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 bahavior 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-Huckle 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, (Willey-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 Mthods*, Ed. W.R. Moser (Academic, San Diago, 1996)

Elective subjects in Organic Chemistry:

2. Polymer Chemistry

Synthesis and Reactions: Scope, definitions, nomenclature, condensation and other Steptype polymerizations - Free radical, ionic and co-ordination polymerizations – Radiation polymerization - Polymerization of cyclic organic compounds - Reactions of synthetic polymers - Biological polymers - Inorganic elements in polymers.
Thermodynamics and Kinetics: Polymerization and depolymerization equilibria - Kinetics of condensation (Step-Growth), Free radical and ionic polymerizations.
Physical Characterization: Molecular wieght (Mn, Mw) determination - Morphology - Glass transitions and crystallinity - Conformational analysis.
Fabrication and Testing: Relationship between structure and properties - Thermal, flame and chemical resistance - Additives - Electroactive polymers - Biomedical applications and biodegradable polymers.

Suggested Reading:

1. H.R. Allcock and F.W. Lampe, Contemporary Polymer Chemistry, Prentice Hall, Inc. (1990).
2. M.P. Stevens, Polymer Chemistry: An Introduction (2nd Edition) Oxford University Press 91990).
3. F.W. Billmeyer, Jr., Textbook of Polymer Science (3rd Edition) Wiley-Inter

Science (1984) paperback.

3. Supramolecular Chemistry

The course will consist of a selection of topics taken from the following aspects of contemporary supramolecular chemistry.
Supramolecular chemistry is the designed chemistry of the intermolecular bond. From molecular to supramolecular structure.
Supramolecular synthesis of organic, metal-organic and inorganic compounds, host-guest chemistry, bioinorganic systems, molecular recognition, replication, self-assembly, solid state assembly, crystal engineering, structure elucidation in the solid state and in solution.
Supramolecular function, catalysis, bioinorganic models, molecular electronic devices, organic conductors, photoresponsive systems, supramolecular electrochemistry, surfactants and interfaces, liquid crystals, biomolecules.

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. Advanced methods in Organic Synthesis

Concepts of symmetrization, umpolung, selectivity and specificity (stereo, regio and chemo). Antithetic and metathetic approaches. Selective introduction and manipulation of functional groups. Selectivity in functional groups reactions, activation, protection and blocking of groups. C-C bond forming reactions-cyanohydrin formation, organometallic additions, Wittig and related reactions, halomethane addition, nucleophilic substitution, Aldol condensation, enolate alkylation, Friedel-Crafts reaction, Michael reaction, Claisen condensation, Cope and Claisen rearrangements, inter- and intra molecular Diel's-Alder reactions, Barbier Weiland degradation, Dieckmann and acyloin condensations, directed aldol condensation, conjugate addition and annulation reactions. Photochemical synthesis. Applications of the above methodologies in the synthesis of key synthones and other molecules.

Text/References

S.Warren, Designing Organic Synthesis, John Wiley and Sons, 1980.
W.Caruthers, Some Methods of Organic Synthesis, Cambridge University Press, 1978.
H.O.House, Modern Synthetic Reactions, 2nd Ed., W.A.Benjamin, 1972.
R.O.C. Norman, Principles of Organic Synthesis, 2nd Edn., Methuen and Co. Ltd., 1972.

5. 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 soon-chemistry, non-conventional reaction media (room temperature ionic liquids, super critical fluids, florous 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 Chgemistry*. Pergamon Press 1994.
7. Gokel, G.W. (Ed) *Advances in Supramolecualr Chemistry*, 2000.
8. Steed, J.W. and Atwood, J.L. Supramolecular Chemistry. Wiley. 2004.