PT. RAVISHANKAR SHUKLA UNIVERSITY

Centre for Basic Sciences

Syllabus of

Integrated M. Sc.: Chemistry Stream

[Choice and Credit Based System]

Semester Examination
SESSION 2015-2020

Center for Basic Sciences
Pt. Ravishankar Shukla University, Raipur

Course structure for the M. Sc. (Integrated) Chemistry stream
1st July, 2015

(B: **B**iology, C: **C**hemistry, M: **M**athematics, P: **P**hysics, G: **G**eneral, H: **H**umanities,
BL: **B**iology **L**aboratory, CL: **C**hemistry **L**aboratory, PL: **P**hysics **L**aboratory,
GL: **G**eneral **L**aboratory, PE: **P**hysics **E**lective, PPr: **P**hysics **Pr**oject)

FIRST YEAR
SEMESTER –I

Subject Code	Subject	Contact Hours / Week Theory +Tutorials	Credits
B101	Biology – I	[2 + 1]	3
C101	Chemistry – I	[2 + 1]	3
M100/101	Mathematics – I	[2 + 1]	3
P101	Physics – I	[2 + 1]	3
G101	Computer Basics	[2 + 1]	3
H101	Communication Skills	[2 + 1]	3
		Contact Hours / Week Laboratory	
PL101	Physics Laboratory – I	[4]	2
CL101	Chemistry Laboratory – I	[4]	2
BL101	Biology Laboratory – I	[4]	2
GL101	Computer Laboratory	[4]	2
			26

(26 of 240 credits)

C 101: Chemistry-I
UNIT-I **(30 + 15 = 45 hrs.)**

Structure and Properties of atoms: Revisited **(4 + 2 = 6 hrs.)**
(i) Atomic spectra, Bohr's theory of atomic structure, Sommerfield's theory for complex electron spin and magnetic quantum number, Pauli exclusion principle, Hund's rule, electron configuration of elements, Sequence of energy levels and Periodic Table.
(ii) Size of atoms and ions, ionization energy, electron affinity, electronegativity – values by Pauling, Mulliken and Allred-Rochow, Metallic character, variable valency and oxidation states, horizontal, vertical and diagonal relationships in the periodic table.

(iii) Atomic Nucleus: Fundamental particles, classification of nuclides, nuclear stability, the neutron to proton ratio N/Z, nuclear potential, binding energy, exchange force. Radioactivity and radioactive elements, radioactive decay and decay kinetics.

UNIT-II

Types of Chemical Bonds (14+ 7 = 18 hrs.)

(i) The covalent bond - the Lewis theory, Octet rule and its limitations. Shapes of the molecules – Sidgwick – powel theory. Valence shell electron pair (VSEPR) theory, effect of lone pair and electronegativity, isoelectronic principle, examples to apply VSEPR theory. Valence bond theory. Hybridization. Bond length, bond angle & dihedral angle, d-orbital participation in molecular bonding, sigma and pi bonding. Molecular orbital method – Linear combination of atomic orbitals (LCAO), MO treatment for di- and tri-atomic molecules and involving delocalized pi-bonding. Conjugation & aromaticity.

UNIT-III

(ii) Metallic and organometallic bonds – general properties.

(iii) Coordinate bond- coordination complexes.

(iv) Physical properties and molecular structures – polaizability and dipole moments, melting point, solubility and acid-base properties, Intermolecular forces (dipole-dipole interaction) Hydrogen bonding and vander Waals's forces.

UNIT-IV

Reactivity & Mechanism: (12 + 6= 18 hrs)

(i) Inductive and field effects and bond dissociation energy. p□-d□ bonding. Delocalization – cross conjugation, resonance. Aromaticity and Huckel's rule – systems of 4n and 4n+2 electrons, antiaromaticity . Resonance and Hyperconjugation.

(ii) Reaction mechanism: Types of mechanisms, Arhenius theory, collision theory, types of reactions, redox reactions, displacement and addition reactions, thermodynamic and kinetic requirements.

UNIT-V

Hammond postulate, Curtin-Hammett principle, transition states and intermediates, carbocations, carbanions, free radicals, methods of determining mechanisms, isotopic effects.

(iii) General concepts: Oxidation number and oxidation states, Oxidation – reduction reactions and the use of reduction potential, Bronsted acids and bases, gas phase vs. solution acidity, solvent levelling effects, hardness and softness, surface acidity.

Suggested texts and References:

(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)R. T. Morrison and R. N. Boyd, Organic Chemistry, Prentice Hall of India.
(5)G.W. Castellan, Physical Chemistry, 3rd Ed. Addison - Wesley/Narosa Publishing House, 1993.

CL 101: Chemistry Laboratory

Calibrations of pipette, burette, standard flasks etc., acid base titrations, recystallization, thin layer chromatography, identification of organic functional groups, complexometric titrations based on EDTA complexation with metals, Synthesis of benzoic acid, diazotization etc.

Suggested text and references:

(1) Vogel's Textbook of Quantitative Chemical Analysis (5th Edition; Longmann)
(2) Vogel's Qualitative Inorganic Analysis (7th Edition)
(3) ACS Journal of Chemical Education

SEMESTER –II

Subject Code	Subject	Contact Hours / Week Theory+Tutorials	Credits
B201	Biology – II	[2 + 1]	3
C201	Chemistry – II	[2 + 1]	3
M200/201	Mathematics – II	[2 + 1]	3
P201	Physics – II	[2 + 1]	3
G201	Electronics and Instrumentation	[2 + 1]	3
G202	Glimpses of Contemporary Science	[2 + 1]	3
		Contact Hours / Week Laboratory	
PL201	Physics Laboratory – II	[4]	2
CL201	Chemistry Laboratory – II	[4]	2
BL201	Physics Laboratory – II	[4]	2
GL201	Electronics Laboratory	[4]	2
			26
			(52 of 240 credits)

C 201: Chemistry II **(30 + 15 = 45 hrs.)**

UNIT-I

(1) Thermochemistry: Enthalpy, heat of fusion and heat of vapourisation, enthalpy of a chemical reaction (heat of combustion, heat of solution, heat of neutralization), enthalpy of formation, standard reaction enthalpy, Hess's law, Kirchhoff's law, bond energy, dissociation energy. Entropy formulation of Second law, entropy change in a phase transition, Trouton's Rule, calculation of absolute (Third law) entropy, entropy change in a chemical reaction.

UNIT-II

(2) Free energy functions, criteria for spontaneity and equilibrium of closed systems, variation of Gibbs free energy with pressure and temperature, Gibbs Helmholtz equation, the concept of chemical potential, partial molar quantity, Gibbs Duhem relation.

UNIT-III

(3) Phase equilibrium in simple systems: Solid – liquid, liquid – vapour, vapour – solid, phase diagrams – water, carbon dioxide, sulphur, phase equilibrium condition, Gibbs phase rule, Clapeyron equations, Clausius – Clapeyron equation.

UNIT-IV

(4) Ideal Solutions, chemical potential of a solute in a binary ideal solution, Raoult's Law, entropy and Gibbs energy of mixing, Colligative properties – freezing point depression, boiling point elevation, osmotic pressure, van't Hoff equation.

UNIT-V

(5) Chemical equilibrium: Gibbs energy change of a reaction, standard reaction Gibbs energy, the condition for chemical equilibrium, equilibrium constant, reactions involving gases and pure substances, the Principle of Le Chatelier and applications.

(6) Chemical potential of a charged species, electrochemical cell (galvanic and electrolytic), examples of electrochemical cells, half cell potential (electrode potential), Nernst equation.

Suggested texts and References:

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

CL 201: Chemistry Laboratory

Colorimetric titrations, Beer Lambert law, Estimation of concentration by colorimetric methods, conductometric methods, estimation of 5oncentration of acid base bt pH meter, identification of inorganic anions and cations, finding of pka values, short project of 2 weeks based on the experiments available in Journal of Chemical Education.

Suggested text and references:

(1) Vogel's Textbook of Quantitative Chemical Analysis (5^{th} Edition; Longmann)
(2) Vogel's Qualitative Inorganic Analysis (7^{th} Edition)
(3) ACS Journal of Chemical Education

SECOND YEAR
SEMESTER –III

Subject Code	Subject	Contact Hours / Week Theory+Tutorials	Credits
CB301	Essential mathematics for Chemistry and Biology	[3 + 1]	4
CB302	Biochemistry-I	[3+ 1]	4
CB303	Organic Chemistry-I	[3 + 1]	4
C301	Inorganic Chemistry-I	[3 + 1]	4
H301	World Literature	[2 + 0]	2
H302	History and Philosophy of Science	[2 + 0]	2
		Contact Hours / Week Laboratory	
CL301	Chemistry Laboratory	[6]	3
GL301	Applied Electronics Laboratory	[4]	2

25

(77 of 240 credits)

CB 303: Organic Chemistry –I **(45 +15 = 60 hrs.)**

UNIT-I

A. Basic concepts - Recapitulation

Hybridisation, formal charge, inductive and resonance effects and their effect on reactivity and acidity and basicity of organic compounds; polar & non polar covalent bonds; homolytic and heterolytic fission, types of reagents- electrophiles and nucleophiles; curly arrow notation; classification of organic reactions.

UNIT-II

B. Chemistry of Aliphatic compounds

IUPAC nomenclature of aliphatic and substituted aliphatic compounds and alicyclic compounds

Preparation, structure, properties and reactions of the following classes of compounds.

i) Hydrocarbons: a) alkanes, Methods of formation Kolbe reaction, Wurtz reaction, Corey House reaction, decarboxylation of carboxylic acids; Mechanism of halogenation of alkanes, orientation, selectivity & reactivity, product ratio. b) **Cycloalkanes** : Methods of formation and reactivity ; Baeyer's strain theory and its limitation; theory of strainless rings c**) Alkenes:**

Elimination reactions ; Saytzeff & Hoffman elimination; Reactions – halogenation reactions-free radical and polar mechanisms. Markownikoff's rule, the peroxide effect, allylic halogenations using NBS; Ozonides/Ozonolysis. epoxidation; hydroboration-oxidation; oxymercuration-demercuration; Oxidation using KMnO4 & OsO4.; polymerization. d**) Dienes:** Structure of butadiene and allene ; 1,2 vs 1,4 addition ; Diels Alder reaction.

UNIT-III

e) Alkynes: Methods of formation; acidity of alkynes; electrophilic addition to alkynes; hydroboration oxidation ; metal ammonia reductions; hydrogenation using Lindlar's catalyst.

ii) Alkyl halides Preparation, properties and synthetic applications of alkyl halides; S_N1 & S_N2 reactions (mechanism), E1 and E2 reactions(mechanism); Grignard reagent and its applications.

iii) Alcohols: Methods of formation; acidity; H-Bonding; reactions of mono; di & trihydric alcohols; Diols as protecting groups.

UNIT-IV

iv) Ethers and epoxides: Formation & reactions of ethers and epoxides ; ring opening reactions of epoxides under acidic and basic consitions; reaction epoxides with Grignard & organolithium reagents

v) Aldehdyes & ketones: Methods of formation of aldehdyes and ketones; Nucleophilic addition reactions with cyanide, ammonia and derivatives of ammonia; acetal formation; oxidation reduction reactions. Meerwin-Pondroff-Verley reduction, Clemmensen reduction, Wolf-Kishner reduction, Aldol condensation reaction, Cannizzaro reaction, Tischenko reaction, haloform reaction, Baeyer-Villiger oxidation, Wittig reaction; Mannich reaction

vi) Carboxylic acids : Methods of formation of mono and di carboxylic acids; acidity and factors affecting acidity; reactions of carboxylic acids :

vii) Carboxylic acid derivatives: Methods of formation of acid chlorides, amides, anhydrides and esters and their interconversions; relative stabilities of acid derivatives; Rosenmund reaction; Hoffmann rearrangement; saponification.

viii) Nitrogen and sulphur compounds. a) Nitro alkanes: methods of formation and reactions of aliphatic and aromatic nitro compounds b) Amines: methods of formation; basicity and factors affecting basicity ; reactions of aliphatic amines. c) Sulfonic acids : Methods of formation & reactions of aliphatic sulfonic acids.

ix) Applications of phosphorous and boron in organic synthesis :

Wittig reaction (with mechanism) ; hydroboration-oxidation (with mechanism); reduction using 9-BBN.

UNIT-V

C. Chemistry of aromatic compounds

IUPAC Nomenclature of benzene, naphthalene and anthracene derivatives

i) Aromaticity: Structure and stability of benzene, Huckel's rule, MO picture, polycyclic aromatic hydrocarbons.

ii) Aromatic electrophilic substitution: General mechanism. Effect of substituents on rate and orientation to aromatic electrophilic substitution in substituted benzenes, ortho-para ratio.

iii) Hydrocarbons: Alkylarenes, preparation via Friedel Crafts reaction. Reactions- oxidation, nuclear and side chain halogenation.

iv) Haloarenes: Preparation, aromatic nucleophilic substitution, elimination-addition and addition-elimination mechanisms, hydrolysis and amination of nitrohaloarenes.
v) Phenols: Preparation from sulfonic acids, haloarenes, alkylbenzenes, Acidity, O-alkylation, O-acylation, Fries rearrangement, Claisen rearrangement, Reimer- Tiemann reaction, Hauben Hoesch reaction, Lederer Manasse reaction.
vi) Aromatic aldehydes and ketones: Preparation via Gattermann, Gattermann-Koch, Vilsmeyer-Haack, Rosenmund and Friedel Crafts acylation reactions, Reactions: Claisen-Schmidt, Knovenagel, Perkin, Benzoin condensation and Cannizaro reactions,
vii) Aromatic carboxylic acids: Preparation, acidity, preparation and interconversion of acid derivatives.
viii) Aromatic sulfonic acids: Preparation, acidity, preparation and interconversion of sulfonic acid derivatives.
ix) Aromatic nitrogen compounds: Nitro and nitroso compounds - preparation and reduction, Amino compounds – preparation, basicity, Aromatic electrophilic substitution, N-alkylation, N-acylation, Diazotisation, Synthetic uses of diazonium salts, azo coupling

Suggested texts and 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) J. March, Advanced Organic Chemistry, 3rd Edn. McGraw Hill,1991.
(7) S.H.Pine, Organic Chemistry, 5th Edn., McGraw Hill, 1987.

C 301: Inorganic Chemistry I

UNIT-I **(45 + 15 = 60 hrs.)**
(i) Hydrogen: Preparation of hydrogen, Isotopes, ortho and para hydrogen, hydrides.
(ii) Rare gases: Occurrence and recovery of the elements, physical and chemical properties, Clathrate compounds, chemistry of Xenon and xenon fluoride complexes.

UNIT-II
(iii) Chemistry of s-block elements: a) alkali and alkaline earth metals: Extraction, general physical properties, flame colours ans spectra, Reaction with water, air and nitrogen, oxides, hydroxides, peroxides and superoxides, sulphides, oxysalts, halides and hydrides, oraganic and organometallic compounds. b) Group IIB elements: Zn, Cd, Hg.

UNIT-III
(iv) Chemistry of p-block elements: a) Group IIIA elements: Boron, aluminium, gallium indium and thalium – physical properties, oxidation states and type of bonds, Reactions with other elements, compounds of boron with oxygen and hydrogen. b) Group IVA elements: carbon, silicon, germanium, tin and lead – physical properties, allotropes of carbon, graphite compounds, carbaides, carbonates, carbon cycle, silicates, organosilicons, hydrides, halides and cyanides, cluster compounds.

UNIT-IV

c) Group VA elements: Nitrogen, phosphorous, Arsenic, antimony and bismuth – general properties, hydrides, azides, oxides and oxyacids, sulphides and organometallics, fertilizers. d) Group VIA elements: oxygen, sulphur, selenium, tellurium and polonium – general properties, structure and allotropy of the elements, chemistry of ozone, oxides, oxyacids, oxohalides, hydrides and halides, organo derivatives.

UNIT-V

e) Group VIIA elements: Fluorine, chlorine, bromine, iodine and Astatine- general properties, oxidizing power, hydrogen halides, ionic and molecular halides, bridging halides, halogen oxides, oxoacids, interhalogen compounds, polyhalides, pseudohalogens and pseudohalides.

Suggested texts and References:

(1) J. E. Huheey, 'Inorganic Chemistry - Principles of Structure and Reactivity' Harper & Row, 1988.
(2) F. A. Cotton and G. Wilkinson, 'Advanced Inorganic Chemistry', John Wiley, 1995.
(3) D. F. Shriver, P.W. Atkins and C.H. Langford, 'Inorganic Chemistry', OxfordUniversity Press, 1991.
(4) F. A.Cotton and G. Wilkinson, Basic Inorganic Chemistry, Wiley Easter, 1978.
(5) J. D. Lee, Concise Inorganic Chemistry, Van Nostrand Reinhold, 1977.

CL 301: Chemistry Laboratory

Experiments of inorganic chemistry: Synthesis of coordination complexes, gravimetric analysis etc

SEMESTER –IV

Subject Code	Subject	Contact Hours / Week Theory+Tutorials	Credits
PCB401	Physical and Chemical kinetics	[3 + 1]	4
CB401	Introductory Spectroscopy (UV-vis, fluorescence, IR, Raman, NMR)	[3+ 1]	4
C401	Properties of Matter	[3 + 1]	4
C402	Group theory	[3 + 1]	4
G401	Statistical Techniques and Applications	[2 + 0]	2
		Lab hrs	**Credits**
CL401	Chemistry Laboratory	[6]	3
GL401	Computational Laboratory and Numerical Methods	[4]	2
			25

(102 of 240 credits)

PCB 401: Physical and Chemical Kinetics: (45 + 15 = 60 hrs.)

UNIT-I

(i) Basic Concepts: Rate, order and molecularity of a reaction, First, second and third order reactions – effect of concentration on reaction rate, rate expressions and integrated form, pseudo-unimolecular and second order autocatalytic reactions, nth order reaction of a single component, effect of temperature on reaction rate – Arrhenius equation and activation energy.

UNIT-II

(ii) Complex Reactions: parallel first order reactions, series first order reactions – determination of rate constants by graphical method and the time ratio method. The stationary state, radioactive decay, general first order series and parallel reactions. Competitive, consecutive second order reactions, reversible reactions, equilibrium from the kinetic view point, complex mechanisms involving equilibria.

UNIT-III

(iii) Kinetic Measurements: Experimental determination of reaction rates and order of reactions – correlation of physical properties with concentrations, reactions in the phase, reactions at constant pressure, fractional-life period method, initial rate as a function of initial concentrations.

UNIT-IV

(iv) Reactions in Solutions: General Properties, Phenomenological theory of reaction rates, Diffusion limited rate constant, Slow reactions, Effect of ionic strength on reactions between ions, Linear free energy relationships, Relaxation methods for fast reactions.

UNIT-V

(v) Catalysis: Homogeneous catalysis in gas phase, in solution, basis of catalytic action, catalysis and the equilibrium constant, acid base catalysis, The Bronsted catalysis law, linear free energy changes, general and specific catalysis. Heterogeneous catalysis. Negative catalysis and inhibition, Surface reactions – effect of temperature and nature of surface. Industrial catalysis.

Suggested texts and References:

(i) K.A. Connors, Chemical Kinetics : A Study of Reaction Rates in Solution, V.C.H. Publications 1990. **(ii)**J.I. Steinfeld, J.S. Francisco and W.L. Hase, Chemical Kinetics and Dynamics, Prentice Hall 1989. **(iii)** Paul L. Houston, Chemical Kinetics and reaction dynamics.
(iv) K.J.Laidler, Chemical Kinetics, 3rd ed. Harper and Row, 1987.
(v) J.W. Moore and R.G. Pearson, Kinetics and Mechanisms, John Wiley and Sons, 1981.
(vi) A. A. Forst and R. G. Pearson, Kinetics and Mechanism, Wiley International Edition.
(vii) Sanjay K. Upadhay, Chemical kinetics and Reaction Dynamics, Springer, 2006

CB401: Introductory Spectroscopy (45 + 15 = 60 hrs)

UNIT-I

(i) The electromagnetic spectrum: Nature of electromagnetic radiation. The electromagnetic spectrum and its regions. Frequency, waveno and wavelength: units and conversions. Absorption of electromagnetic radiation. Molecular energy states and quantisation of internal energy. Boltzmann distribution.

(ii) Spectroscopic Processes: Absorption, emission, and scattering of light. Beer-Lambert Law - Quantitative absorption measurements, Jablonski diagram
(iii) Fourier transformation: A mathematical tool to our advantage, basic principle and its relevance in spectroscopy.

UNIT-II

(iv) UV-VIS Absorption Spectroscopy: Principles and instrumentation of spectrophotometers. UV-vis spectroscopy to determine conjugation. UV-visible spectroscopy and electronic transitions. Electronic ground states and excited states in organic molecules: n to pi-star and pi to pi-star transitions. band position and band intensities.
(v) Fluorescence Spectroscopy: Principles and instrumentation of fluorimeters. Advantage of fluorimetry compared to absorption spectrophotometry. Luminescence and the fate of excited states: timescale of fluorescence and phosphorescence.Qualitative and Quantitative Fluorimetry.
UNIT-III

(vi) IR - Principles and instrumentation of Infrared spectroscopy. nfrared spectroscopy and molecular vibrational transitions. Simple dispersive IR spectrometer and ovewrview of modern instrumentation. Transmittance and absorbance. Vibrational modes and selection rules. Factors governing the position and intensity of IR bands: effects of variation in reduced mass and force constant. Group frequency and fingerprint regions: use of IR for identification by presence/absence of absorptions characteristic of specific bonds/bond groupings. Interpretation of IR spectra.
(vii) Raman Spectroscopy: Raman Effect and molecular polarizability. Technique and instrumentation. Pure rotational Raman spectra, vibrational Rama spectra. Structure determination from Raman and IR.

UNIT-IV
(viii) Nuclear Magnetic Resonance (NMR): Introduction to Nuclear Magnetic Resonance (NMR) spectroscopy. 1H and 13C NMR, number of signals, integration, chemical shift, splitting of signals. Principles and instrumentation of NMR spectroscopy. Nuclear spin and nuclear magnetism. Energies of nuclear spin states in a magnetic field. Boltzmann population of nuclear spin states and the origin of NMR signals. Applications: Interpretation of simple 1H NMR spectra. Information from: chemical shifts and delta values, peak areas and integration, splitting patterns and spin-spin coupling constants. (n+1) rule and Pascal's triangle. 13C NMR spectra and sensitivity issues. Interpretation of NMR spectra using examples of organic compounds. Short introduction about application of NMR for proteins.

UNIT-V

(ix) Mass spectrometry: Introduction to mass spectroscopy (molecular mass, accurate mass and isotopes) Principles, ionisation methods (including EI, MALDI, ESI). Molecular ions and fragmentation processes under EI. Mass spectrometry for determining the molecular weight/formula of organic compounds and identify the presence of isotopes. Introduction of MS application in protein analysis.

C 401: Properties of Matter **(45 + 15 = 60 hrs.)**

UNIT-I

(i) Gaseous State a). 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. b). 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. c). 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. d). Collision number and mean free path, transport properties: viscosity, thermal conductivity and diffusivity of gases.

UNIT-II

(ii) The Liquid State: a) Intermolecular forces – dipole-dipole London forces, hydrogen bonding. b) Vapour pressure, determination of vapour pressure, external and internal pressure, boiling point and vapour pressure. c) 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. d) Viscosity, measurement of relative and absolute viscosity, viscosity and temperature, molecular weight from viscosity. e) refractive index, specific rotation, molar refraction and chemical constitution, optical activity and specific rotation.

UNIT-III

(iii) 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. Ionic, covalent, metallic and coordinate bonds. (ii) Ionic Bond - characteristics of ionic compounds and crystal structures, radius ratio rules and coordination number, close packing. Classification of ionic structures – AX, AX2 and AX3 groups. Lattice Energy, Stoichiometric defects – Schottky and Frenkel. Non-stoichiometric defects – metal excess and metal deficiency. Semiconductors and transistors.

UNIT-IV

(iv) 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.

UNIT-V

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, Ideal solution and colligative properties.

Suggested texts and References:

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

C 402: Group theory (45 + 15 = 60 hrs)

UNIT-I

(i) Symmetry Elements and Operations, Pure Rotations (C_nRotations), Improper Rotations, Rotation-Reflection (S_n) & Rotation-Inversion (n-bar) Axes.

UNIT-II

(ii) Point Groups: Low Symmetry Point Groups (C1 ,Ci , Cs), Simple Axial Point groups (c., S4n, Cnv' Cnh), Dihedral Groups (Dn, , Dnd, Dnh)

UNIT-III

Platonic Solids & the "Cubic" Groups (Td, 0h , Ih), Derived High Symmetry Groups (T, Th , 0, I), The "Infinite Groups" (C∞v and D∞h), Points Groups & Chirality, Point Groups & Dipole Moment.

UNIT-IV

(iii) 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.

UNIT-V

(iv) 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.

Suggested texts and References:

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

G 401: statistical techniques and its applications

CL 401: Chemistry Laboratory

Acetylation of primary amine, synthesis of cyclohexanone oximes, nitration of phenols, bromination of acetanilide, photoreduction of benzophenone to benzopinacole, pinacole pinacolone rearrangements, benzil- benzilic acid rearrangement, aldol condensation, coenzyme catalysed benzoin condensation, separation of organic mixtures(solid-solid, solid -liquid and liquid-liquid), characterization of all the synthesized compounds using FTIR, UV-vis spectroscopy and 1H-NMR**.**

3rd Year

SEMESTER –V

Subject Code	Subject	Contact Hours / Week Theory+Tutorials	Credits
CB501	Analytical Chemistry	[3 + 1]	4
C501	Quantum Chemistry	[3+ 1]	4
C502	Inorganic Chemistry II	[3 + 1]	4
C503	Organic Chemistry II	[3 + 1]	4
G501	Earth Science and Energy & Environmental Sciences	[3 + 1]	4
		Lab contact hrs	**Credits**
CL501	Chemistry Laboratory	[8]	4
			24

(126 of 240 credits)

CB 501: Analytical Chemistry **(45 + 15 = 60 hrs.)**

UNIT-I

(i) Error analysis: Methods of sampling and associated errors, Classification of errors, Propagation of errors, treatment of errors, Normal distribution, Tests of Significance and Confidence Limits.

UNIT-II

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

UNIT-III

(iii) Mass Spectrometry: Mass Analysers – Magnetic, Quadrupole, Time of Flight (TOF), Features – Resolution, Dispersion, Abundance, Sensitivity, Detectors, Ion Sources –Thermal Ionisation (TI), Electron Impact, ICP, GD, Laser Ablation (LA-ICP), Secondary Ionisation (SI),

Matrix Assisted Laser Desorption and Ionisation (MALDI), Hyphenated Technique – IC-MS, HPLC-MS, GC-MS.

UNIT-IV

(iv) Thermal Methods: Thermogravimetric Analysis (TGA), Derivative Thermogravimetric Analysis (DTG), Differential Thermal Analysis (DTA), Differential Scanning Calorimetry (DSC), Evolved Gas Analysis (EGA).
(v)Electrochemical Methods: Introduction, Potentiometry , Ion Selective Electrodes (ISE), Voltammetry & Polarography , Cyclic, Pulse and Stripping Voltammetry, Coulometry and Amperometry, AC Electrochemical Techniques, Scanning Electrochemical Microscopy.
(vi) 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.

UNIT-V

(vii) Conductance of solutions and electrochemistry: Faraday's laws of electrolysis, Electrolytic conduction- Arrhenius theory of electrolytic dissociation, strong and weak electrolytes. Migration of ions – transference numbers, Determination of transference number using 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.

Suggested texts and References:

(1) D.A. Skoog, D. M. West, F. J. Holler, S.R. Crouch, Fundamentals of Analytical Chemistry, 8th Edition, Thomson (2004).
(2) 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).
(3) A. K. De, S. M. Khopkar and R. A. Chalmers, Solvent Extraction of Metals, Van Nostrand, Reinhold (1970).
(4) L. R. Snyder and J. J. Kirkland, Introduction to Modern Liquid Chromatography, 2nd Edition, Wiley (1979).
(5)Jose A. C. Broekaert, Analytical Atomic Spectrometry with flames and Plasmas, Wiley-VCH (2002).
(6) John Roboz, Introduction to Mass Spectrometry: Instrumentation and Techniques, Interscience (1968).

C 501: Quantum Chemistry (45 + 15 = 60 hrs.)
UNIT-I

(i) Foundations of quantum mechanics.
(ii) Wave function for a free particle, the Schrodinger equation, physical interpretation of the Scrodinger equation wave function, expectation of a dynamical quantity, Wavepackets and the uncertainty principle, WKB approximation.

UNIT-II

(iii) Operator concept in quantum chemistry.
(iv) 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.

UNIT-III

(v) Approximate methods of quantum chemistry: variational principle; Time-independent perturbation theory: Many electron sysytems: Orbital approximation, Slater determinant; Hartree-Fock self-consistent field theory; Slater type orbitals.

UNIT-IV

Concept of LCAO and introduction to ab-initio and semi-empirical molecular orbital calculations of molecules. Huckel Theory: Extended systems: From bonds to bands. Angular momentum of many-particle systems. Born-Oppenheimer approximation, MO and VB theories illustrated with H2-molecule, An elementary treatment of scattering theory.

UNIT-V

(vi)Spin orbital interaction; LS and JJ coupling. Spectroscopic term symbols for atoms. Molecules and Chemical bonding, Spectroscopic term symbols for diatomics; Directed valence & hybridization in simple polyatomic molecules.

Suggested texts and References:

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

C 502: Inorganic Chemistry II: (45 + 15 = 60 hrs.)
UNIT-I

(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, □-complexes, □-acid ligands, multiple bonds from ligands to metals.

UNIT-II

(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.

UNIT-III

(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.

UNIT-IV

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.

UNIT-V

(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.

Suggested texts and 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*

C 503: Organic Chemistry – II **(45 + 15 = 60 Hrs.)**

UNIT-I

(A) Stereochemistry of Organic Compounds 25h **(i)** Isomerism – Concept and types **(ii)** Chirality: Configuration, stereogenic/chiral center, chirality and enantiomerism. Representation of configuration by flying wedge formulae and Fischer, Newman and Sawhorse projection formulae. **(iii)** Stereochemistry of carbon compounds with upto three similar and dissimilar asymmetric carbon atoms; enantiomers, diastereomers, and racemic mixtures and their properties, resolution (chemical and chromatographic). **(iv)** Diastereomerism: Threo, erythro, meso diastereomers. Geometrical isomerism in olefins, cycloalkanes and oximes. Absolute

configuration: Assigning of stereochemical descriptors - R/S to Fischer projection and flying wedge formulae of chiral molecules and E/Z to olefins.

UNIT-II

(v) Molecular chirality and elements of symmetry: Stereochemistry and stereochemical nomenclature of biphenyls, spirans, cummulenes, and alkylidene cycloalkanes **(vi)** Conformational concepts, conformations of acyclic molecules (ethane and butane), cyclohexane and mono, di-substituted cyclohexanes. Conformationally rigid and mobile diastereomers. **(vii)** Stereoselectivity and stereospecificity of organic reactions: Enantiomeric and diastereomeric selectivities.

UNIT-III

The mechanism and stereochemical outcome of the following reactions: (a) S_N1, S_N2 and S_Ni reactions (b) Catalytic hydrogenation of alkenes (c) Ionic trans addition of bromine to alkenes (d) Epoxidation of alkenes, acid catalysed ring opening of epoxides. (e) Reactions of OsO_4 and $KMnO_4$ with olefins (f) E2 reactions. (g)Topicity and prostereoisomerism - Enantiotopic and diastereotopic atoms, groups and faces.

UNIT-IV

(B) Chemistry of heterocyclic compounds **25h**

Heterocycles containing one heteroatom (furan, thiophene, pyrrole, pyridine) and more than one heteroatom (pyrazole, imidazole, oxazole, thiazole, pyrimidine and pyrazines) their derivatives – preparation, properties and reactions. **(C) Chemistry of Alicyclic compounds:** Cycloalkanes and cycloalkenes. Factors affecting stability of conformations, conformation of cycloalkanes. Reaction mechanism in alicyclic compound.

UNIT-V

(i) Conformation of Cyclic System: Monocyclic compounds and Fused ring and Bridged ring Compound. Topicity and Prostereoisomerism & Racemisation and Methods of Resolution.

(ii) Dynamic stereochemistry: Conformationally rigid and mobile diastereomers, seteroselectivity.

(iii) Chemistry of Carbon radical (Single electron transfer mechanism): neighboring group participation; non-classical carbocataion; S_Ni mechanism. Rearrangements of Carbocataion, Free-radical: Allylic, Pinacol/ Pinacolone, 1,2 rearrangements etc and rearrangement to heteroatoms. Pericyclic reaction and FMO approach.

Suggested texts and 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.F.G. Riddell, The Conformational Analyis of Heterocyclic Compounds, Academic Press, 1980.

(4) L.A. Paquette, Principles of Modern Heterocyclic Chemistry, W.B. Benjamin, Inc., 1978.

(5) B.M. Acheson, An Introduction to the Chemistry of Heterocyclic Compounds, Interscience, 2nd Ed., 1975.

G501: Earth Science and Energy & Environmental Sciences

Earth Science

Origin of the earth, type of rocks in different layers, their physical and chemical properties, mechanism of their formation and destruction. Radioactivity and its role in geochronology, Plate tectonics and geodynamics and the role of mantle plumes in sustaining these processes. Gravity, electrical and magnetic properties of the different layers in the earth. Their variations in different geological terrains. Instrumentation, field procedures used in these studies. Response of the earth to the elastic (Seismic) and electromagnetic waves, use of this phenomena to study the earth's interior. Geodynamo and the internal magnetic field of the earth. Paleomagnetic studies, Polar wandering and reversal, possible theoretical arguments for understanding the phenomena. Seismology and its use in understanding of the different layers in the earth's interior. Utility of the different geophysical techniques (discussed above) in exploration for academic as well as for harnessing resources.

Suggested Texts and references:

1. The magnetic field of the Earth, Merill, R.T. McElhinny, M.W. and McFadden, P.L. International Geophysical Series.
2. Earth Science by Edward J. Tarbuck, E.J. and Lutgens, F.K.
3. Introduction to Applied Geophysics: Exploring the Shallow Subsurface Burger, H.R., Sheehan, A.F., C.H.
4. Mantle Plumes and Their Record in Earth History, Condie, K.C., 2001, Cambridge University Press, Cambridge, UK
5. Applied Geophysics (Paperback) W M Telford, Robert E Sheriff and L P Geldart.

Energy and Environmental Sciences

Introduction to Environmental Science. Natural Environments: Ecosystems and ecology, biodiversity. Socio-cultural environments: demography, population density, human organizations. Land use and its planning. Global climate change and effects on environment. Carbon cycle from human activity, calculation of carbon budgets. Water harvesting, storage and treatment. Natural calamities, hazards, and effects of human activity: Chemical and other technological hazards. Various case studies of natural calamities and human-induced disasters. Causes, effects, forecasting, preparedness, planning measures, technological solutions, social interventions. Concept of sustainability, individual and social, and local and global actions for a sustainable future. Introduction to energy Sources - evolution of energy sources with time. Power production, per capita consumption in the world, and relation to development index. Energy scenario in India: Various issues related to consumption and demands -energy crisis issues in India. Renewable and non-renewable energy sources - technology and commercialization of energy sources, local (decentralized) versus centralized energy production, constraints and opportunities of renewable energy (hydrocarbon and coal based energy sources). Energy conservation – calculation of energy requirements for typical and home and industrial applications. Alternative to fossil fuels - solar, wind, tidal, geothermal. Bio-based fuels. Hydrogen as a fuel. Energy transport and storages, comparison of energy sources - passage from source to delivery (source, production, transport, delivery) - efficiencies, losses and wastes. Nuclear energy: Power production: Components of a reactor and its working, types of reactors and comparison. India's three stage nuclear program. Nuclear fuel cycle. Thorium based reactors. Regulations on nuclear energy.

Suggested texts and References:

1. Energy in Perspective, J.B.Marion, University of Maryland, Academic Press, (1974)
2. Energy and Environment, Robert A.Ristinen and Jack J. Kraushaar, 2nd Edn., John Wiley and
Sons, Inc. (2006).
3. Renewable Energy, Boyle Godfrey, Oxford University Press (2004)
4. Environment, Problems and Solutions, D.K.Asthana and Meera Asthana, S.Chand and Co.(2006)
5.Text Book on Environmental Chemistry, Balaram Pani, I.K.International Publishing House(2007).

CL 501 Chemistry Laboratory:

Isolation and purification of lysozyme protein from hen egg by different methods (ethanol, ammonium sulfate and TCA precipitation), Relative quantification of lysozyme obtained from different methods by using:Dialysis, Gel electrophoresis, UV-Vis spectroscopy, Purification of lysozyme obtained from different methods with fast performance liquid chromatography (FPLC), Qualitative analysis of the lysozyme obtained after FPLC by using spectroscopic techniques (UV-Vis and fluorescence spectroscopy), Calculation of Quantum yield using fluorescence Spectroscopy, Binding effect of ligand on fluorescence of protein fluorophore (Calculation of inner filter effect), Calculation of binding constant of a ligand with protein by Stern-Volmer plot using fluorescence spectroscopy, Study of solvent effects on the stability of proteins by drawing a denaturation profile in presence of denaturing agents using UV-Vis and fluorescence spectroscopy.

SEMESTER –VI

Subject Code	Subject	Contact Hours / Week Theory+Tutorials	Credits
CB601	Biophysical Chemistry	[3 + 1]	4
C601	Atomic and molecular spectroscopy	[3+ 1]	4
C602	Inorganic Chemistry III	[3 + 1]	4
C603	Organic Chemistry III	[3 + 1]	4
C604	Nuclear Chemistry	[3 + 1]	4
H601	Ethics in Science and IPR	[2 + 0]	2
		Lab contact hrs	**Credits**
CL601	Chemistry Laboratory	[6]	3
			25

(151 of 240 credits)

CB 601: Biophysical Chemistry

UNIT-I

(i) The Chemistry of Life: An introduction: Physical properties of water: Structure, water as solvent, The hydrophobic effect, osmosis and diffusion. Introduction to Biomolecules: Nucleic

Acid, Protein - Polymer Description of Macromolecular Structure, Intermolecular and Intramolecular forces, Non Covalent Interaction

.

UNIT-II

(ii) General principles of Biophysical chemistry I: Hydrodynamic properties: Diffusion and sedimentation, determination of molecular weight from sedimentation and diffusion; Introduction of Ultra Centrifugation, Dynamic Light Scattering and Electrophoresis. Spectroscopic properties of proteins and nucleic acid: UV/Vis, Intrinsic fluorescence, Circular dichroism.

UNIT-III

(iii) General principles of Biophysical chemistry II: The concept and application of Chemical and Physical equilibria in Biological system, The equilibrium constant and Standard Gibbs Free energies of reactants and products, Temperature dependence of the equilibrium constant, Double Strand formation in nucleic acid, Ligand-protein binding, Protein denaturation and stability, Introduction of DSC and ITC.

UNIT-IV

(iv) Molecular self-assembly and Molecular medicine: Protein folding kinetics and Biophysical methods, Misfolding and aggregation; Physical basis of conformation diseases, Therapeutic approaches to protein misfolding diseases**.**

UNIT-V

(v) Introduction to structure biology: Introduction to basic principles of protein X-ray crystallography, protein NMR, Small Angle X-ray scattering (SAXS), and Electron microscopy (EM).

Suggested texts and References:

(1) Tinoco, Sauer, Wang, and Puglisi. (2003) Physical Chemistry: Principles and Applications in the Biological Sciences. Prentice Hall, Inc.

(2) Physical Chemistry for the Life Sciences: Peter Atkins and Julio de Paula

(3) General review papers Dobson CM. Principles of protein folding, misfolding and aggregation. Semin Cell Dev Biol. 2004 Feb;15(1):3-16.

C 601: Atomic and molecular Spectroscopy (45 + 15 = 60 hrs.)

UNIT-I

(i) Born-Oppenheimer approximation - rotational, vibrational and electronic energy levels of homonuclear and heteronuclear diatomic and polyatomic molecules.

UNIT-II

(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.

UNIT-III

(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.

UNIT-IV

(iv) Raman Spectroscopy: Classical and quantum theories of Raman effect and molecular polarizability. Pure rotational Raman spectra, Vibrational Raman spectra, Polarization of light and the Raman effect, Structure determination from Raman and infrared spectroscopy, Techniques and Instrumentation, Near IR FT Raman spectroscopy. Resonance Raman and electronic Raman transition and applications.

UNIT-V

(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.

Suggested texts and References:

(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.

C 602: Inorganic Chemistry III (45+15 = 60 hrs)

UNIT-I

Chemistry of d-block elements

(i) General introduction to transition elements – Electronic structure, Metallic character, variable oxidation state, complexes, magnetic and catalytic properties.

UNIT-II

(ii) Elements of the first transition series: Occurance, separation, extraction and chemistry of the scandium group (IIIB), titanium Group (IVB), vanadium group (VB), chromium group (VIB), Manganeese group (VIIB).

UNIT-III

Iron group (VIIIB(8)), Nickel group (VIII(9)) and Copper group (VIIIB(10)).

(iii) Chemistry of the elements of the second and third transition elements: fnium group (Group IVB), Niobium and Tantalum (Group VB), Molybdenum and tungsten (Group VIB); Technitium and Rhenium (Group VIIB),

UNIT-IV
The Platinum group Metals, Ruthenium and Osmium (Group VIII(8)); Rhodium and Irridium (Group VIII(9)), Palladium and Platinum (Group VIII(10), Silver and gold Group (1B(11)).

UNIT-V
(iv)Chemistry of f-block elements-The lanthanide and actinide elements.

Suggested texts and References:
(1) Advanced Inorganic Chemistry, F. Albert Cotton and G. Wilkinson@1988, John Wiley & Sons.

C 603: Organic chemistry III (45 + 15 = 60 Hrs.)

UNIT-I
Chemistry of Natural Products:
(i) Terpenoids: Classification, structure, chemistry and biogenesis of some important mono; sesqui,di, and triter penes.

UNIT-II
(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.

UNIT-III
(iii) Alkaloids: Characteristic reactions, general methods of degradation, structure and chemistry of some well-known alkaloids.

UNIT-IV
(iv) Natural Pigments: anthocyanines, Flavones, flavanones, isoflavones, xanthones, quinones, pterins, chlorophyll and haemin.

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

Suggested texts and References:
(1) I. L. Finar, Organic Chemistry, Vol. 1 & 2, ELBS.

C 604: Nuclear Chemistry (45 + 15 = 60 hrs.)

UNIT-I
(i) 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.

UNIT-II

(ii) Modes of Decay: □ decay, □ decay, electron captures, □ de-excitation, internal conversion, artificial radioactivity.

(iii) 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.

UNIT-III

(iv) Applications of radioactivity: Probing by isotopes, preparation of radioisotopes, Szilard-Chamers' reaction, Concept of tracers, chemical yield, radiochemical purity, Application of radiotracers in Chemical Sciences, uses of nuclear radiations, radioisotopes as a source of electricity.

UNIT-IV

(v) Elements of Radiation Chemistry: Interaction of radiation with matter, radiation dosimetry, radiolysis of water and some aqueous solutions, other radiolytic events.

(vi) Nuclear Methods: Activation Analysis – Neutron Activation Analysis (NAA),

UNIT-V

Charged Particle Activation Analysis (CPAA), X-ray fluorescence (XRF) spectrometry, Ion Beam Analysis – Backscattering Spectrometry (BS), Particle Induced □-ray Emission (PIGE), Nuclear Reaction Analysis (NRA), Elastic Recoil Detection Analysis (ERDA), Particle Induced X-ray Emission (PIXE).

Suggested texts and 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).

H601: Ethics of Science and IPR

Introduction to a Collective, Participatory Teaching-learning Program: A Science of Our own. Science Stands the Test of Ethics … Some indicators. Levels of Moral Development - Does it mean anything?

Medical Ethics: Different themes pertaining to medical ethics including ethical issues in public health.

History, Philosophy and Psychology of Ethics: History of Political Economy and Modern Ethics Environmental Ethics

Intellectual Property Rights and Associated Issues: History of Patenting. Digitalizing Culture-I: Free Software and Free Culture. Digitalizing Culture-II: Concentration and appropriation of Power by the few as well as Possibility of Distributive Justice

Journals and Publishers: Monopolistic practices by Academic Publishers Quest for Determining what is Virtuous: Ethics in Practice. Collaborative Projects by the Class.
Teaching the Teachers and other Virtuous Inquiries.

CL 601: Chemistry laboratory:
Experiments based on analytical techniques such as cyclic voltammetry, pulse polarography, electrodeposition, gas chromatography, nuclear magnetic resonance, FTIR, thermal gravimetry methods, atmic absorption spectroscopy etc.

FOURTH YEAR
SEMESTER –VII

Subject Code	Subject	Contact Hours / Week Theory+Tutorials	Credits
C701	Photochemistry	[3 + 1]	4
C702	Chemical biology	[3+ 1]	4
C703	Organometallics & Bio-inorganic Chemistry	[3 + 1]	4
C704	Physical Organic Chemistry	[3 + 1]	4
CPr701	Reading project	-	4
		Lab contact hrs	**Credits**
CL701	Advanced Chemistry Laboratory-I	[8]	4
			24

(175 of 240 credits)

C701: Photochemistry **(45 + 15 = 60 hrs.)**

UNIT-I
Basic Principles of photochemistry:
(i) 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.
(ii) Properties of the excited state: Acid-base properties, redox potential, geometry, dipole moment, dynamic properties of the excited states.

UNIT-II
(iii) 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.

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

UNIT-III

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

UNIT-IV

(vi) 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.

UNIT-V

(vii) 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 dn complexes, photochemistry of carbonyl compounds, energy conversion (solar) and photodecomposition of water.

Suggested texts and 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 702: Chemical Biology (45 + 15 = 60 Hrs.)

UNIT-I

(i) Structure and the Synthesis of Life: Central Dogma, Introduction to Biological Chemistry, Artificial gene synthesis: solid-phase DNA synthesis Versus molecular cloning and polymerase chain reaction (PCR). Synthia and *Mycoplasma laboratorium,*

UNIT-II

DNA digital data storage, Peptide and protein synthesis. Lipid synthesis,Carbohydrate and membrane synthesis.

What Chemists Can Do for Biology: Natural Versus non Natural amino acid, Nonnatural Amino Acids for Site-Specific Protein Conjugation, Bio-orthogonal chemistry, Chemical genetics, reverse chemical genetics.

UNIT-III

Biomimetic Chemistry: Compounds that mimics a biological material in its structure or function, Artificial Enzymes: Chemical transformation, Molecular recognition (Mimic binding), examples of mimics found in research and industry: Cyclodextrins Cryptands,

UNIT-IV

Catalytic antibodies. Nanozymes- next-generation artificial enzymes, A laboratory procedure designed to imitate a natural chemical process: Biomimetic synthesis, Natural product synthesis, Asymmetric catalysis, Reaction methodology.

UNIT-V

(iv) Metabolomics: Technologies in metabolomics. Nutrigenomics. Other omics. Nuclear Magnetic Resonance Spectroscopy and Mass Spectrometry in metabolomics. Metabolic pathways resources: KEGG, Biocarta. Nutrigenomics and metabolic health. Solved problems and future challenges.

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

UNIT-I

Organometallics: Overview, 18-electron rule, square planar complex. Carbonyl ligand – bonding, binary carbonyl complexes, oxygen-bonded carbonyls, other ligands similar to CO, IR spectrum, main group parallels with binary carbonyl. Pi-ligands – linear and cyclic pi systems, NMR spectra of organometallic complexes.

UNIT-II

Comparative survey of structure and bonding of metal alkyls and aryls, complexes with 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.

UNIT-III

importance of organometallic compounds in certain biological systems. Other important ligands – complexes containing M – C, M= C, M ≡ C bonds, hydride and dihydrogen complexes, phosphines and related ligands.

(ii) 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.

UNIT-IV

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.

UNIT-V

(iii) Bio-inorganic 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.

Suggested texts and References:

(1) G.O.Spessard, G.L.Miessler, Organometallic Chemistry, Prentice Hall, 1997.
(2) C.Elsehenbroich and A. Salzer, Organometallic Chemistry, 2nd Ed., Wiley VCH, 1992.
(3) F.A.Cotton, G. Wilkinson, C.A. Murillo and M. Bochmann, Advanced Inorganic Chemistry, 6th Edn., Wiley, 1999.
(4) N.N.Greenwood and A. Earnshaw, Chemistry of the Elements, lst Edn., Pergamon, 1985.
(5) S.J.Lippard & J.M.Berg, Principles of bioinorganic chemistry, University Science Books, Mill Valley, 1994.
(6) I. Bertini, H.B.Gray, S.J.Lippard and J.S.Valentime, Bioinorganic Chemistry, Univ. Sci. Books, Mill Valley, 1994.
(7) James A.Cowan, Inorganic Biochemistry, VCH Publishers, 1993.

C 704: Physical organic chemistry (45 + 15 = 60 hrs)

UNIT-I

Structure and Models of Bonding: Basic Bonding Concepts, Bonding and Structure of Reactive Intermediates, Molecular Orbital Theory, electron in a box problem, energies and coefficients of linear pi-systems, Secular Determinant, Huckel MOT, HMOT in cyclic and acyclic pi-systems, Aromatic and antiaromatic systems.

UNIT-II

(ii) Strain and Stability: Thermochemistry of Stable Molecules, Thermochemistry of Reactive Intermediates, Relation Between Structure and Energetics-Basic Conformational Analysis, Conformations of Acyclic and Cyclic Systems, Electronic Effects.

Acid-Base Chemistry: Bronsted Acid-Base Chemistry, Aqueous and Non-Aqueous Systems, Predicting Acid Strength in Solution, Lewis Acids/Bases and Electrophiles/Nucleophiles.

UNIT-III

(iv) Thermal Pericyclic Reactions: Cycloadditions, Orbital correlation diagram, Frontier Molecular Orbital, Comments on forbidden and allowed reactions, Photochemical pericyclic reactions, D-A cycloadditions, regio- and stereoselectivity, endo-effect, [2+2] cycloaddition, ketene cycloaddition, 1,3-dipolar cycloaddition, ene-reaction, retrocycloaddition, electrocyclic

reactions, torquoselectivity, sigmatropic rearrangements, Claisen and Cope rearrangements, Cheletropic reactions.

UNIT-IV

(v) Reactivity, Kinetics and Mechanisms: Energy Surfaces and Related Concepts, Postulates and Principles Related to Kinetic Analysis, Kinetic Experiments and Deciphering Mechanisms. **(iv)Experiments Related to Thermodynamics and Kinetics:** Isoptope Effects, Substituent Effects, Hammett Plots and Linear Free Energy Relationships, Other Linear Free Energy Relationship, Acid-Base Related Effects, Experiments for Studying Mechanism.

UNIT-V

(vii) Application of physical methods: Deciphering mechanisms of electrophilic and nucleophilic substitution/additions, eliminations, cyclizations, radical reactions and reactions involving reactive intermediates.

Suggested texts and References:

(1) E. V. Anslyn and D. A. Dougherty, Modern Organic Chemistry, University Science, 2005.
(2) I. Fleming, Molecular Orbitals and Organic Chemical Reactions, John Wiley, 2009.
(3) J. Clayden, S. Warren, N. Greeves, P. Wothers, Organic Chemistry, 1st Edition, Oxford University Press, 2000
(4) F. J. Carey and R. J. Sundburg, Advanced Organic Chemistry, Part A and Part B, 5th Ed., Springer, 2007
(5) J. March, Advanced Organic Chemistry, 3rd edition, McGraw Hill, 1991.
(6) S. H. Pine, Organic Chemistry, 5th edition, McGraw Hill, 1987.

SEMESTER –VIII

Subject Code	Subject	Contact Hours / Week Theory+Tutorials	Credits
C801	Chemistry of Materials	[3 + 1]	4
C802	Macro and Supra-molecular chemistry	[3+ 1]	4
C803	Reaction Dynamics	[3 + 1]	4
C804	Computational Chemistry	[3 + 1]	4
		Lab contact hrs	**Credits**
CL801	Advanced Chemistry Laboratory-II	[10]	5
CPr801	Project	-	4
			25

(200 of 240 credits)

C801: Chemistry of Materials **(45 + 15 = 60 hrs.)**

UNIT-I

Basic Aspects of the Solid State

(i) Solid State Structure: Primitive lattice vectors - reciprocal lattice - crystal systems and desymmetrization schemes. Bravais lattices; closed packed structures, octahedral and tetrahedral holes, crystallographic point groups and space groups - organic and in organic crystal structure motifs - polytypes and polymorphs. pervskites and related structures, normal and inverse spinels.
(ii) Defects and Non-stoichiometry: Intrinsic and extrinsic defects - point, line and plane defects; vacancies, Schottky defects, Frenkal defects - Charge compensation in defective solids - non-stoichiometry, thermodynamic aspects and structural aspects.

UNIT-II

(iii) 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.
(iv) 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.

UNIT-III

(v) 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.
(vi) Magnetic Properties: Classification of magnetic materials - Langevin diamagnetism - Quantum theory of paramagnetism - cooperative phenomena - magnetic domains and hysteresis - magnetism and dimensionality.
(vii) Optical Properties: Optical reflectance - excitons - Raman scattering in crystals - photoconduction - color centers - lasers - photovoltaic effect.

UNIT-IV

(viii) Synthesis of Materials: Phase diagrams - preparation of pure materials, mass transport, nucleation and crystal growth - preparative techniques, zone refining, chemical transport, etc.
(ix) 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.
(x) Nanocrystalline phase - preparation procedures – special properties - applications
(xi) 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.

UNIT-V

(xii) 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.
(xiii) Materials for Solid State Devices: Rectifiers, transistors, capacitors - IV-V compounds - low-dimensional quantum structures, optical properties.
(xiv) Organic Solids, Fullerenes, Molecular Devices: Conducting organics – organic superconductors - magnetism in organic materials.
(xv) Fullerenes - doped fullerenes as superconductors
(xvi) Nonlinear Optical Materials: Nonlinear optical effects, second and third order – molecular hyperpolarisability and second order electric susceptibility - materials for second and third harmonic generation.

Suggested texts and 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).
(4) Charles Kittle, Introduction to solid state physics, John Wiley & Sons, New York (1968). Anthony R.West, Solid State Chemistry and its Applications, John Wiley & Sons, New York (2005).
(5) Lesley E. Smart, Elaine A. Moore, Solid State Chemistry (3rd Ed), Taylor & Francis (2005).
(6) N.N. Greenwood, Ionic crystals, lattice defects and non-stoichiometry,

C 802: Macro and Supramolecular Chemistry (45 + 15 = 60 hrs.)

UNIT-I
A. Polymer Chemistry
(i) Polymerization reactions, mechanism and kinetics – cationic, anionic and radical polymerization. Template, emulsion and electrochemical polymerization, Condensation, ring opening, step growth and radiation polymerization reactions. Coordination complex polymerization, Naturally occurring polymers, Biological polymers, inorganic polymers. Polymerization of cyclic organic compounds. Copolymerization and multicomponent polymerization,
(ii) Thermodynamics and kinetics. Polymerization and depolymerization equilibria - Kinetics of condensation (Step-Growth), Free radical and ionic polymerizations.

UNIT-II
(iii) Physical Characterization: Fabrication and Testing, Relationship between structure and properties - Thermal, flame and chemical resistance - Additives - Electroactive polymers - Biomedical applications. Molecular wieght (Mn, Mw) determination - Morphology -Glass transitions and crystallinity - Conformational analysis. Dynamics of dilute polymer solutions and effect of increasing concentration, NMR and neutron scattering studies.
(iv) Reactions and degradation of polymers, biodegradable polymers. Thermal and oxidative degradation, catalysis by macromolecules, computer applications.

UNIT-III

Supramolecular Chemistry

(i) Introduction to Supramolecular Chemistry.

(ii) Molecular and Chiral Recognition - Self-Organization, Self-Assembly and Preorganization, molecular and chiral recognition, self-Assembly and self-organization, role of preorganization in the synthesis of topological molecules, template reactions, one-pot' reactions.

(iii) Covalent self-assembly based on preorganization - inclusion complexes, host-guest chemistry, early development of host-guest chemistry. pedersen's works onc crown ethers, nomenclature, the structure of inclusion complexes, dynamic character of inclusion complexes, the complexes involving induced fit and without it, endo-hedral fullerene, hemicarcerand and soft rebek's tennis ball-like hosts.

(iv) Mesoscopic Structures as an Intermediate Stage Between Molecules (Micro Scale) on the One Hand and Biological Cells (Macro Scale) on the Other – introduction, medium sized molecular aggregates.

UNIT-IV

(v) Between Classical Organic Chemistry and Biology Understanding and Mimicking Nature-Introduction, the role of self-organization and self-association in the living nature, modeling processes in living organisms.

(vi) On the Border Between Chemistry and Technology - Nanotechnology and Other Industrial Applications of Supramolecular Systems – introduction, between chemistry and solid state physics - crystal engineering, obtaining crystals with desired properties, nanotechnology and other industrial applications of supramolecular systems, supramolecular catalysis.

(vii) The Most Interesting Macrocyclic Ligands which Are Hosts for Inclusion Complexes- . Crown ethers and coronands, cryptates and cryptands, calixarenes, hemispherands, and spherands, carcerands, hemicarcerands and novel `molecular flasks' enabling preparation and stabilization of short-lived species, cyclodextrins, and their Complexes, endohedral fullerene complexes, nanotubes and other fullerene-based supramolecular systems, dendrimers, cyclophanes and steroids forming inclusion complexes, anion binding receptors and receptors with multiple binding Sites.

UNIT-V

(viii) Other Exciting Supramolecular Systems- Making Use of the preorganization phenomenon, topological molecules, multiple hydrogen-bonded Ssstems, organic zeolite, metal directed self-assembly of comple, supramolecular architecture, chains, racks, ladders, grids, macrocycles, cages, nanotubes and self-Intertwining strans (helicates).

(ix) The Prospects of Future Development of Supramolecular Chemistry.

Suggested texts and References:

1. H.R. Allcock, F.W. Lampe and James Mark, 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.

4. A. Ravve, Principles of Polymer Chemistry.

5. Recommended Review Articles in the field of supramolecular chemistry.

6. "Supramolecular Chemistry" by F. Vogtle, John Wiley, 1991.
7. "Crystal Engineering. The Design of Organic Solids" by G.R. Desiraju, Elsevier, 1989.
8. Introduction to Supramolecular Chemistry, Dodzuick Helena.

C 803: Reaction dynamics (45 + 15 = 60 hrs.)

UNIT-I

Chain reactions: general treatment, activation energy, chain length, chain transfer reactions, inhibition, bond dissociation energies, branching chain reactions.

UNIT-II

The collision theory: Dynamics of bimolecular collisions and rate and rate constant of bimolecular reaction, factors determining effectiveness of collisions, Termolecular reactions, unimolecular reactions. Relation between cross section and rate coefficients.

UNIT-III

Potential Energy Surfaces:: Long range, empirical intermolecular and molecular binding potentials, Internal coordinates and normal modes of vibration, Potential energy surfaces, ab-initio calculation of potential energy surface, experimental determination of potential energy surfaces.

UNIT-IV

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

UNIT-V

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

Suggested texts and References:

(1) J.I. Steinfeld, J.S. Francisco and W.L. Hase, Chemical Kinetics and Dynamics, Prentice Hall 1989.
(2) Paul L. Houston, Chemical Kinetics and reaction dynamics.
(3) R.D.Levine and R.B.Bernstein, Molecular Reaction Dynamics and Chemical Reactivity, Oxford University Press, 1987.
(4) Sanjay K. Upadhay, Chemical kinetics and Reaction Dynamics, Springer, 2006

C 804 Computational chemistry (45 + 15 = 60 hrs.)

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.

Suggested texts and References:

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

FIFTH YEAR
SEMESTER –IX

Subject Code	Subject	Contact Hours / Week	Credits
CPr901	Project	-	24
			24

(224 of 240 Credits)

SEMESTER –X

Subject Code	Subject	Contact Hours / Week Theory+Tutorials	Credits
CE1001	Elective I	[3 + 1]	4
CE1002	Elective II	[3+ 1]	4
CE1003	Elective III	[3 + 1]	4
CE1004	Elective IV	[3 + 1]	4
			16

(240 of 240 credits)

(P: Physics, M: Mathematics, C: Chemistry, B: Biology, G: General, E: Elective, Pr: Project)

Elective subjects on Physical Chemistry:

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.

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

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(Xnn (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.

Environmental Chemistry

Biocycles: C, O2, N2, P, S, CO2, 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

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 99Mo-99mTc generators; Few other important generator systems such as 90Sr-90Y, 188W-188Re etc. Methods of production of some important radioisotopes (such as 32/33P, 41Ar, 60Co, 79Kr, 82Br, 90Sr-90Y, 99Mo-99mTc, 125I, 131I, 137Cs, 153Sm, 166Ho, 177Lu, 186/188Re, 192Ir, and 11C, 13N, 15O, 18F, 67Ga, 123/124I, 201Tl 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.

Advanced techniques in NMR spectroscopy

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.

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
1.W.L.Jolly, Modern Inorganic Chemistry, McGraw, Hill Co., 1984.
2.R.W. Hay, Bioinorganic Chemistry, Wiley, 1984.

3.M.Day and J.Selbin, Theoretical Inorganic Chemistry, Von. Nostrand, 2nd Ed. 1980.
4.H.J.Emeleus and J.J. Anderson, Modern Aspects of Inorganic Chemistry, Von. Nostrand, 1962.
5.J.E.Huheey, Inorganic Chemistry, 4th Ed., Harper Collins College Publisher, 1993.
6.G.H.Stout and L.H.Jensen, X-ray Structure Determination : A Practical guide, 2nd Ed., John Wiley, 1989.

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

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

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.

2.5 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.
2.6 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.

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)

Advanced Coordination Chemistry

A. Advanced Coordination Chemistry 25 hrs.

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

Text/References

1. R.S.Drago, Physical Methods for Chemists, W.B. Saunders Co., 1992.
2. B.N.Figgis, Introduction to Ligand Fields, Wiley Eastern, 1976.
3. A.B.P. Lever, Inorganic Electronic Spectroscopy, Elesevier, 1968.

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.

■