MASTER OF SCIENCE IN CHEMISTRY

SYLLABUS FOR THE CREDIT BASED CURRICULUM

FROM 2013 ONWARDS

Department of Chemistry
National Institute of Technology
Tiruchirappalli – 620 015

M.Sc. Chemistry

Code	Course of Study	L	T	P	C
SEMESTER 1					
CH 601	Organic Chemistry - Reaction Mechanisms and Their Types	3	-	-	3
CH 603	Coordination Chemistry: Bonding, Reactions and Spectra	3	-	-	3
CH 605	Quantum Chemistry and Group Theory	3	-	-	3
CH 607	Instrumental Methods of Chemical Analysis	3	-	-	3
CH 609	Organic Preparations and Separations Lab	-	-	6	2
CH 611	Inorganic Preparations and Qualitative Analysis Lab	-	-	6	2
	ELECTIVE I	**3**	**-**	**-**	**3**
		-	**-**	**-**	**19**
SEMESTER II					
CH 602	Photochemistry, Pericyclic and Rearrangement Reactions	3	-	-	3
CH 604	Organometallic and Bioinorganic Chemistry	3	-	-	3
CH 606	Thermodynamics, Electrochemistry and Kinetics	3	-	-	3
CH 608	Molecular Spectroscopy	3	-	-	3
CH 610	Physical Chemistry Lab	-	-	6	2
CH 612	Analytical Chemistry Lab	-	-	6	2
	ELECTIVE II	**3**	**-**	**-**	**3**
		-	**-**	**-**	**19**
SEMESTER III					
CH 613	Synthetic Organic Chemistry	3	-	-	3
CH 615	Solid State, Nuclear and Main Group Chemistry	3	-	-	3
CH 617	Statistical Thermodynamics, Photochemistry and Surface Chemistry	3	-	-	3
CH 619	Fundamentals and Applications of Spectroscopy	3	-	-	3
CH 621	Organic and Inorganic Quantitative Analysis Lab	-	-	6	2
CH 623	Computational and Spectroscopy Lab	-	-	6	2
	ELECTIVE III	**3**	**-**	**-**	**3**
		-	-	-	19
SEMESTER IV					
CH 614	M.Sc. Project	-	-	20	10
	Total Credits	**-**	**-**	**-**	**67**

ODD SEMESTER ELECTIVES

Code	Course of Study	L	T	P	C
CH 625	Catalysis	3	-	-	3
CH 627	Environmental Chemistry	3	-	-	3
CH 629	Inorganic Rings, Cages and Clusters	3	-	-	3
CH 631	Medicinal Chemistry	3	-	-	3
CH 633	Nano Science and Technology	3	-	-	3
CH 635	Nuclear Chemistry	3	-	-	3

EVEN SEMESTER ELECTIVES

Code	Course of Study	L	T	P	C
CH 616	Computational Methods in Chemistry	3	-	-	3
CH 618	Natural Products Chemistry	3	-	-	3
CH 620	Polymer Chemistry	3	-	-	3

CH 601 - Organic Chemistry - Reaction Mechanisms and Their Types

Reaction mechanism: Definition of reaction mechanism, transition state theory, kinetics, qualitative picture. Substituent effects, linear free energy relationships, Hammett equation and related modifications. Basic mechanistic concepts like kinetic *vs* thermodynamic control, Hammond postulate, Curtin-Hammett principle, isotope effects, general and specific acid-base catalysis, and nucleophilic catalysis.

Nucleophilic substitution: Reactivity, structural and solvent effects, substitution in S_N1, S_N2, S_Ni. Neighbouring group participation -Norbornyl and bridgehead systems, substitution at allylic and vinylic carbons, substitution by ambident nucleophiles, aromatic nucleophilic substitution, S_N Ar, benzyne, S_N1. Aromatic nucleophilic substitution of activated halides

Addition to carbon-carbon multiple bonds: Electrophilic, nucleophilic and free radical addition. Stereochemistry and orientation of the addition. Hydrogenation, halogenation, hydroxylation, hydroboration. Addition to carbonyl compounds - 1,2 and 1,4-addition, benzoin, Knoevenegal, Stobbe and Darzen glycidic ester reactions.

Elimination reactions: E1, E2, E1CB- mechanism, stereochemistry, orientation of double bonds - Hoffmann, Zaitsev, Bredts rule - pyrolytic elimination, Chugaev reaction. Oxidation and reduction: Reduction using hydride reagents, $LiAlH_4$, $NABH_4$ and other organoboranes: chemo- and stereoselectivity, catalytic hydrogenation (homogenous and heterogeneous catalysts), Swern and Dess-Martin oxidations, Corey-Kim oxidation, PCC, $KMnO_4$ oxidations.

Theories of aromaticity: Aromaticity, antiaromaticity, Huckel's rule, annulences and heteroannulenes, fullerenes (C60). Other conjugated systems, Chichibabin reaction. Aromatic electrophilic substitution: Orientation, reactivity, and mechanisms. Substitution in thiophene and pyridine. Reactive intermediates - carbenes, nitrenes, radicals, Ylides - Formation, stability and their applications.

References:

1. M. B. Smith, J. March, March's Advanced Organic Chemistry, John Wiley & Sons, 6th Edn, 2007.
2. R. R. Carey and R. J. Sundburg, Advanced Organic Chemistry, Part A and Part B, Springer, 5th Edn, 2007.
3. Peter Sykes, A Guide Book to Mechanism in Organic chemistry, Orient-Longmens, 6th Edn, 1996.
4. E. J. Eliel, Stereochemistry of Carbon Compounds, John Wiley, 1997.
5. P. Y. Bruice, Organic Chemistry, Pearson Education, 3rd edition, 2006.

CH 603 - Coordination Chemistry: Bonding, Reactions and Spectra

Theories of coordination compounds - VB theory - CFT - splitting of d orbitals in ligand fields and different symmetries - CFSE - factors affecting the magnitude of 10 Dq - evidence for crystal field stabilization - spectrochemical series - site selection in spinels - tetragonal distortion from octahedral symmetry - Jahn-Teller distortion - Nephelauxetic effect - MO theory - octahedral - tetrahedral and square planar complexes - π-bonding and molecular orbital theory - experimental evidence for π-bonding.

Reactions: Substitution reactions in square planar complexes - the rate law for nucleophilic substitution in a square planar complex - the trans effect - theories of trans effect - mechanism of nucleophilic substitution in square planar complexes - kinetics of octahedral substitution - ligand field effects and reaction rates - mechanism of substitution in octahedral complexes - reaction rates influenced by acid and bases - racemization and isomerization - mechanisms of redox reactions - outer sphere mechanisms - excited state outer sphere electron transfer reactions - inner sphere mechanisms - mixed valent complexes.

Electronic spectra and magnetism: Microstates, terms and energy levels for $d^1 – d^9$ ions in cubic and square fields - selection rules - band intensities and band widths - Orgel and Tanabe-Sugano diagrams - evaluation of 10 Dq and β for octahedral complexes of cobalt and nickel - charge transfer spectra - magnetic properties of coordination compounds - change in magnetic properties of complexes in terms of spin orbit coupling - temperature independent paramagnetism - spin cross over phenomena.

IR and Raman spectroscopy: Structural elucidation of simple molecules like N_2O, ClF_3, NO_3^-, ClO_4^- - effect of coordination on ligand vibrations - uses of group vibrations in the structural elucidation of metal complexes of urea, thiourea, cyanide, thiocyanate, nitrate, sulphate and DMSO - effect of isotopic substitution on the vibrational spectra of molecules - applications of Raman spectroscopy

Structure: Structure of coordination compounds with reference to the existence of various coordination numbers (2, 3, 4, 5 & 6) - site preferences - isomerism - trigonal prism - absolute configuration of complexes - stereo selectivity and conformation of chelate rings - coordination number seven and eight. Spectral and magnetic properties of lanthanide and actinide complexes.

References:

1. J. E. Huheey, E. A. Keiter and R. L. Keiter, Inorganic Chemistry, Principles of Structure and Reactivity, 4th Edition, Harper Collin College Publishers, 1993.
2. F.A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, 4th & 5th Edns, Wiley Interscience, New York, 1998.
3. R.S. Drago, Physical Methods in Inorganic Chemistry, 3rd Edition, Wiley Eastern, 1992.
4. J. Lewis, R.G. Wilkins, Modem Coordination Chemistry, Inter Science Publisher, 1960.
5. D. F. Shriver, P. W. Atkins and C. H. Langford, Inorganic Chemistry, Oxford University Press, Oxford, l994.
6. K. Nakamoto, Infrared and Raman Spectra of Inorganic and Coordination Compounds, Part A & Part B, 2nd Edn, Wiely. 2009
7. G. L. Miessler, D. A. Tarr, Inorganic Chemistry, 3rd Edn, Pearson Prentice Hall, 2005
8. J. E. House, Inorganic Chemistry, Elsevier, 2008.

CH 605 - Quantum Chemistry and Group Theory

Quantum chemistry-I: The failures of classical physics – Black body radiation - photoelectric effect - Bhor's quantum theory, Wave particle duality - Uncertainty principle- Operator algebra, Linear and Hermitian operators, Quantum mechanical postulates, Schrodinger equation and its solution to the problem of a particle in one and three dimensional boxes.

Quantum chemistry-II: Quantum mechanical results for a rigid rotator and simple harmonic oscillator, Solution of Schrodinger equation for harmonic oscillator and rigid rotor. Schrodinger equation for hydrogen atom and its solution - Derivation of Eigen function and Eigen value for hydrogen atom. Term symbols for electronic state in atoms – LS and JJ coupling. The origin of electronic quantum numbers and physical significance - radial probability density - significance of magnetic quantum number with respect to angular momentum.

Quantum chemistry-III: Hydrogen molecule ion and hydrogen molecule - Pauli's exclusion principle. Born Oppenheimer approximation, Mulliken designation of molecular orbitals. MO theory of bonding, MO treatment of H-bonded systems, ethylene, butadiene and benzene. Approximation methods: Perturbation and variation method, wave functions for many electron atoms – Hartree-Fock SCF method, Slater orbitals.

Group theory-I: Elements of group theory, definition, group multiplication tables, conjugate classes, conjugate and normal subgroups, symmetry elements and operations, point groups, assignment of point groups to molecules, Matrix representation of geometric transformation and point group, reducible and irreducible representations, construction of character tables, bases for irreducible representation, direct product, symmetry adapted linear combinations, projection operators. Orthogonality theorem - its consequences.

Group theory-II: Symmetry aspects of molecular orbital theory, planar π-systems, symmetry factoring of Huckel determinants, solving it for energy and MOs for ethylene and 1,4-butadiene, sigma bonding in AX_n molecules, hybridization, tetrahedral, octahedral, square planner, trigonal planar, linear, trigonal bipyramidal systems, hybrid orbitals as linear combination of AOs, electronic spectra, selection rule, polarization electron dipole transition, electronic transitions in formaldehyde, butadiene, configuration interaction, vibrational spectra, symmetry types of normal molecules, symmetry coordinates, selection rules for fundamental vibrational transition, IR and Raman activity of fundamentals in CO_2, H_2O, N_2F_2, the rule of mutual exclusion and Fermi resonance.

References:

1. I. N. Levine, Quantum Chemistry, 4th Edn., Prentice Hall India, 1994.
2. A. K. Chandra, Introductory Quantum Chemistry, Tata McGraw Hill, 1994.
3. M. S. Gopinathan and V. Ramakrishnan, Group Theory in Chemistry, Vishal Publishers, 1988.
4. D. A. McQuarrie, Quantum Chemistry, University Science Books, 1983.
5. F. A. Cotton, Chemical Applications of Group Theory, 2nd Edn., Wiley Eastern Ltd., 1990.
6. R. K. Prasad, Quantum Chemistry, TMH, 1995.
7. P.W. Atkins, Physical Chemistry, 6th Edn., Oxford University Press, 1998.

CH 607 - Instrumental Methods of Chemical Analysis

Errors in chemical analyses: Terms and definitions - systematic errors. Random errors - statistical treatments - standard deviation of calculated results and reporting computed data - statistical data treatment and evaluation: Confidence intervals, statistical aids to hypothesis testing - analysis of variance and detection of gross errors.

Separation techniques: Solvent extraction - Methods of extraction and applications of solvent extraction. Solid phase extraction - methods and applications – chromatography - thin layer chromatography, ion exchange chromatography and size exclusion chromatography – HPLC - outline study of instrument modules. Gas chromatography – basic instrumental set up - carriers, columns, detectors and comparative study of TCD, FID, ECD and NPD. Theory & applications – electrophoresis - theory and applications.

Electrochemical techniques: Potentiometry - electrode systems, direct potentiometric titrations - null-point potentiometry and applications - polarography, stripping voltammetry & amperometric techniques - diffusion currents, Half-wave potentials, construction & characteristics of the DME - quantitative analysis - amperometric titrations and applications of polarography – electrogravimetry and coulometry - coulometry at constant potential, coulometric titrations - conductometric titrations.

Atomic spectrometry: Atomic absorption spectrometry (AAS) - absorption of characteristic radiation, instrumentation - Hollow cathode lamp - sampling - quantitative measurements and interferences - atomic emission - instrumentation, plasma sources – instrumentation - inductively coupled plasma - mass spectrometry (ICP–MS) - principles & instrumentation and applications of flame emission spectrometry - flame characteristics & processes - applications of flame photometry and flame atomic emission spectrometry.

Thermal techniques: Elemental analysis – CHNSO - thermogravimetry - instrumentation and applications of TG. Differential thermal analysis (DTA) - instrumentation and applications of DTA. Differential scanning calorimetry (DSC) - Instrumentation, applications of DSC and comparison of DTA & DSC. Thermomechanical analysis (TMA) and dynamic mechanical analysis (DMA) - instrumentation, applications of TMA and dynamic mechanical analysis.

References:

1. G. H. Geeffery et al., Vogel's Text Book of Quantitative Chemical Analysis, ELBS Edn, 1989.
2. D. A. Skoog, D.M. West, F.J Holler, S.R Crouch, Fundamentals of Analytical Chemistry, 8th edition, Thomson Brooks Cole, 2004.
3. F. Rouessac and A. Rouessac, Chemical Analysis: Modern Instrumentation Methods and Techniques, 2nd edn, John Wiely and Sons.
4. D. A. Skoog, E. J. Holler, S. R. Crouch , Principles of Instrumental Analysis, 6th edition, Thomson Brooks Cole , 2007.
5. F. W. Fifield and D. Kealey, Principles and Practice of Analytical Chemistry, 2nd Edition, International Book Company, London, 1983.
6. H. H. Willard, L.L. Merrit, J.A. Dean and F.A. Settle, Instrumental Methods of Analysis, D, CBS Publishers, New Delhi, 1986.

CH 609 - Organic Preparations and Separations lab

(a) **Preparations** - Double stage preparation of m-nitrobenzoic acid from methyl benzoate, preparation of acetyl salicylic acid from methyl salicylate, preparation of triacetoxy benzene from hydro quinone, preparation of m-nitroaniline from nitro benzene, preparation of tribromo benzene from aniline, preparation of p-nitroaniline from acetanilide. Single stage preparations involving acetylation, alkylation, condensation, hydrolysis, esterification etc.
(b) **Extraction** - Extraction of caffeine from tea leaves.
(c) **Chromatography** - Separation of anthocyanidine from hibiscus rosasinens, separation of sugars, separation of amino acids.
(d) Separation and characterization of two component and three component mixtures.

References:

l. A. I. Vogel, Text Book of Practical Organic Chemistry, 5th Edn., ELBS, London, l989.
2. B. B. Dey and M. V. Sitharaman, Laboratory Manual of Organic Chemistry, Revised by T.R. Govindachari, Allied Publishers Ltd., New Delhi, 4th Revised Edn., l992.

CH 611 - Inorganic Preparations and Qualitative Lab

Semi-micro analysis (minimum 8 mixture): Analysis of mixture containing two common cations and any two of the following less familiar cations. Tl, W, Se, Te, Mo, Ce, Th, Ti, Zr, V, Be, U and Li.
Synthesis and characterization of any five Compounds:
Potassium trioxalato cobaltate
Bromopentammino cobalt chloride
Tris(ethylenediammine)chromium(III) chloride
Hexammine cobalt(III) chloride
Tris(ethylenediammine)cobalt(III) chloride
Cis and trans dichlorobis(ethylenediammine)cobalt(III) chloride and resolution of the cis form
Hexammine nickel(II) bromide
Bis(NN'-bis(o-hydroxybenzylidine)ethylenediamine)-m-aquodicobalt(II)
Dichloro(di-2-pyridylamine)copper(II) and Bis(Di-2-pyridylamine)copper(II)chloride
Bis(ethylenediamine)nickel(II) chloride
Tris(acetylacetonato)iron(III)
Tris(acetylacetonato)manganese(III)

References:

1. Manual provided by the department.
2. V.V., Ramanujam , Inorganic Semi-micro Qualitative Analysis, 3rd Edn., National Publishing Company, Madras, l990.
3. G. Brauer (Ed.), Handbook of Preparative Inorganic Chemistry, Vols. I and II, Academic Press, 1963.

CH 602 - Photochemistry, Pericyclic and Rearrangement Reactions

Fundamentals of photochemistry: Qualitative introduction about different transitions, cis-trans isomerization, Paterno-Buchi reaction, Norrish type I and II reactions, photo reduction of ketones, photochemistry of arenes, di-pi-methane and Hoffmann-Loeffler-Freytag rearrangements.

Pericyclic reactions: Classification, electrocyclic, sigmatropic, cycloaddition and ene reactions, Woodward-Hoffmann rules, and FMO theory, Claisen, Cope, Sommelet-Hauser, and Diels-Alder reactions in synthesis, stereochemical aspects.

Optical activity and chirality: absolute and relative configuration - R-S notation system, molecules with more than one asymmetric center. Enantiotopic and diastereotopic atoms, groups and faces. Stereo specific and stereo selective synthesis, optical isomerism of biphenyls, allenes and spiranes. Compounds containing chiral nitrogen and sulfur. Geometrical isomerism, E, Z- nomenclature of olefins, cumulenes and oximes.

Conformational analysis: Fischer projection, inter-conversion of Sawhorse, Newman and Fischer projections, conformational analysis of ethane and disubstituted ethane derivatives, cycloalkanes and substituted cyclohexane. Conformation and stereochemistry of cis and trans decalin and 9-methyldecalin. Anomeric effect in cyclic compounds.

Rearrangement reactions: involving electron deficient, carbon, nitrogen, oxygen centers, emphasis on synthetic utility of these rearrangements. Baker–Venkataraman, benzilic acid, [1,2]-Meisenheimer, [2,3]-Meisenheimer, Wagner-Meerwein, Pinacol, Demyanov, Dienone-Phenol, Favorskii, Wolff, Hofmann, Curtius, Lossen, Schmidt, Beckmann, Benzidine, Hofmann-Loffler rearrangements.

References:

1. House, Modern Synthetic Reactions, 1973.
2. R.O.C. Norman and J. M. Coxon, Principles of Organic Synthesis, ELBS, 1994.
3. J. J. Li, Name Reactions, Springer, 3rd Edn, 2006.
4. B. P. Mundy, M. G. Ellerd, F. G., Jr. Favaloro, Name Reactions and Reagents in Organic Synthesis, Wiley-Interscience, 2005.

CH 604 - Organometallic and Bioinorganic Chemistry

Structure and bonding in organometallics: 18/16-electron rule - metal carbonyls – bonding – spectra – nitrosyls - dinitrogen complexes – phosphines - metal alkyls, aryls, hydrides and dihydrogen complexes - π-bonding ligands – metallocenes - electronic structure and bonding in ferrocene - synthesis, physical and spectroscopic properties of metallocenes - fluxional molecules.

Reaction mechanism and catalysis: Ligand substitution - oxidative addition and reductive elimination - 1,1 and 1,2-insertion - addition and elimination reactions - alkene isomerization-hydroboration - hydrocyanation - hydrogenation of olefins - Wilkinson's catalyst - hydroformylation of olefins - Wacker-Smidt synthesis - Monsanto acetic acid process - Eastman Halcon process - Fischer-Tropsch process - hydrosilylation.

Carbenes: Fischer and Schrock carbenes - bonding & reactivity - Grubbs catalyst - carbynes structure, synthesis and reactions - alkene metathesis – mechanism - RCM-ROMP, SHOP and ADMET - C-H and C-C activation - agostic bonds - Ziegler-Natta polymerization of olefins - Heck reaction - The Pauson Khand reaction - Ene reaction.

Transport of metal ions: Uptake, transport and storage of metal ions by organisms - structure and functions of biological membranes - the generation of concentration gradients (the Na^+-K^+ pump) - mechanisms of ion-transport across cell membranes – bleomycin - siderophores (e.g. enterobactin and desferrioxamine) - transport of iron by transferring - storage of iron by ferritin - bio chemistry of calcium as hormonal messenger.

Metalloporphyrins/Metalloenzymes: Dioxygen transport and storage - hemoglobin and myoglobin: electronic and spatial structures - hemeythrin and hemocyanine - synthetic oxygen carriers, model systems - blue copper proteins (Cu) - iron-sulfur proteins (Fe)-cytrochromes electron transport chain - carbon monoxide poisoning - iron enzymes - peroxidase, catalase and cytochrome P-450, copper enzymes - superoxide dismutase, vitamin B12 and B12 coenzymes, photosynthesis - photosystem-I & II, nitrogen fixation, cisplatin.

References:

1. R.H. Crabtree, The Organometallic Chemistry of Transition Metals, 4th Edn Wiley-VCH.
2. G.O. Spessard and G. L. Miessler, Organometallic Chemistry, 2nd Edn, Oxford University Press.
3. S. J. Lippard & J. M. Berg. Principles of Bioinorganic Chemistry, Panima Publ. Corpn. (2005).
4. W. Kaim & B. Schwederski. Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, John Wiley (1994).
5. J. E. Huheey, E. A. Keiter and R. L. Keiter, Inorganic Chemistry, Principles of Structure and Reactivity, 4th Edition, Harper Collin College Publishers, 1993.
6. J. P. Collman, Principles and Applications of Organotransition Metal Chemistry, Standford University.
7. S. E. Kegley and A. R. Pinhas, Problems and Solutions in Organometallic Chemistry, University Science Books.
8. C. Elschenbroich, Organometallics, 3rd Edn, Wiely VCH.
9. J. F. Hartwig, Organotransition Metal Chemistry: From Bonding to Catalysis, 1st Ed, University Science Books, 2010.

CH 606 -Thermodynamics, Electrochemistry and Kinetics

Thermodynamics: Third law, thermodynamics, need for it, Nernst heat theorem and other forms of stating the third law. Thermodynamic quantities at absolute zero, apparent exceptions to the third law - thermodynamics of systems of variable composition, partial molar properties, chemical potential, relationship between partial molar quantities, Gibbs Duhem equation and its applications (the experimental determination of partial molar properties not included) - thermodynamic properties of real gases, fugacity concept, calculation of fugacity of real gas, activity and activity coefficient, concept, definition, standard states and experimental determinations of activity and activity coefficient of electrolytes.

Phase rule, colloids and micelles: Phase rule: Three component systems, representation by triangular diagrams, systems of three liquids, formation of one pair of partially miscible liquids, formation of two pairs of partially miscible liquids, solid, liquid phases, eutectic systems - colloids: Distinction between suspension, colloidal solutions and true solutions, lyophilc and lyophobic colloids, Tyndall effect, stability of colloids, coagulation, emulsions, various types. Micelles: Surfactant (amphipathic molecule), micellisation, critical micelle concentration, size of micelle, aggregation number, thermodynamics of micellization, solubilisation behavior of micelles, reverse, micelles.

Electrochemistry-I: Ion transport in solution - migration, convention and diffusion -Fick's laws of diffusion conduction - influence of ionic atmosphere on the conductivity of electrolytes - The Debye Huckel-Onsager equation for the equivalent conductivity of electrolytes - experimental verification of the equation - conductivity at high field and at high frequency - conductivity of non aqueous solutions - effect of ion association on conductivity. The electrode-electrolyte interface - electrical double layer - electro capillary phenomena - Lippmann equation - the Helmholz - Perrin - Guoy - Chapmann and Stern models, electrokinetic phenomena Tiseiius method of separation of protons of proteins - membrane potential.

Electrochemistry-II: Elecrodics - mechanism of electrode reactions - polarization and over potential - the Butler volmer equation for one step and multistep electron transfer reaction - significance of equilibrium exchange current density and symmetry factor -significance of transfer coefficient - mechanism of the hydrogen evolution reaction and oxygen evolution reactions. Some electrochemical reactions of technological interest - corrosion and passivity of metals - construction and use of Pourbaix and Evans diagrams - methods of protection of metals from corrosion, fuel cells - electro deposition.

Chemical kinetics: Simultaneous reactions - opposing, parallel and consecutive reactions, the steady state approximation - theories of reaction rates - transition state theory and collision theory a comparison - enthalpy, entropy and free energy of activation, potential energy surfaces, reaction coordinates, kinetic isotope effects, factors determining reaction rates in solution, solvent dielectric constant and ionic strength. Chain reactions - linear reactions, branching chains - explosion limits; Rice–Herzfeld scheme; kinetics of free radical polymerization reactions. Enzyme catalysis - rates of enzyme catalysed reactions - effect of substrate concentration, pH and temperature - determination of Michael's parameters.

References:

1. S. Glasstone, Thermodynamics for chemists, Affiliated East West Press, 1965.
2. Atkins, P.W. 'Physical Chemistry', 6th Edn., Oxford University Press, 1998.
3. K. J. Laider, 'Chemical Kinetics', 3rd Edn., Harper and Row Publishers, 1987.
4. J. O. M. Bockris and A. K. N. Reddy, Modern Electrochemistry, Plenum Press, 1970.
5. J. Rajaram & J. C. Kuriacose, Thermodynamics for Students of Chemistry, Shobanlal Nagin Chand Co, 1986

CH 608 - Molecular Spectroscopy

Electromagnetic radiation: its interaction with matter - Einstein coefficients - time dependent perturbation theory - transition probability - transition dipole moments - energy levels in atoms and molecules – Born-Oppenheimer approximation - selection rules - intensity and width of spectral lines - Fourier transformation.

Rotational spectra: Diatomic and polyatomic molecules - selection rules, rotational Raman spectra - vibrational spectra of diatomic molecules - rotational character of vibration spectra - morse potential of real molecules - selection rules - overtones and combination - Fermi resonance.

Vibrational spectra: Polyatomic molecules - harmonic and anharmonic oscillators - Morse potential - selection rules - normal modes of vibrations of polyatomic molecules - selection rules - Fourier transformation in IR spectroscopy - Raman spectroscopy – fundamentals - rotational Raman - vibrational Raman spectra - IR/ Raman instrumentation.

Electronic spectroscopy: Atoms and molecules - term symbols - Frank Condon principle - vertical transitions - selection rules - parity, symmetry and spin selection rules - polarization of transitions - fluorescence and phosphorescence - Russell Sanders coupling - different types of electronic transitions - electronic spectra of conjugated systems - transition metal complexes - UV-Vis instrumentation - circular dichorism – ORD – applications - surface plasmon resonance - dynamic light scattering.

Electron spectroscopy: Photoelectric effect, basic principles of electron spectroscopy, classification - electron energy analysis - photon sources - UV, X-ray, synchrotron, theory, angular dependence - cross section and its determination - valence and core photoemission - Koopmans' theorem - Introduction to ESCA - Auger electron spectroscopy - EXAFS.

References:

1. C. N. Banwell, Fundamentals of Molecular Spectroscopy, 4th edn. Tata McGraw Hill, 1996.
2. J. M. Hollas, Modern Spectroscopy, 4th Edn, John Wiley & Sons, 1992.
3. P. F. Bernath, Spectra of Atoms and Molecules, 2nd Edn, Oxford University Press, 2005.
4. D. C. Harris and M. D. Bertolucci, Symmetry and Spectroscopy, Dover, 1989.
5. P. K. Ghosh, Introduction to Photoelectron Spectroscopy, Wiley Interscience, 1983.

CH 610 - Physical Chemistry Lab

1. Kinetic study of hydrolysis of ester. Determination of order, I^- and $S_2O_8^{2-}$.
2. Kinetics of iodination of acetone by spectrophotometer.
3. Partition coefficient of NH_3 between water and chloroform.
4. Determination of partition coefficient and equilibrium constant for $KI + I_2 \rightarrow KI_3$.
5. Adsorption of oxalic acid on activated charcoal.
6. Determination of heat of solution and heat of fusion.
7. Study of three component system.
8. Determination of solubility product.
9. Study of chain linkages in PVA and its molecular weight determination by viscometry.
10. Partial molar volume of NaCl.
11. Buffer preparation and pH-metric titration.
12. Conductometric titration of mixture of acids and precipitation titration (KCl *Vs* $AgNO_3$) using conductivity bridge.
13. Potentiometric titrations.
14. Determination of the capacitance of electrochemical interfaces, formal potential and diffusion coefficient of $[Fe(CN)_6]^{3-}$ by cyclic voltammetry.
15. Estimation of Pb^{2+} ion by amperometric titration.

References: Manual provided by the department.

CH 612 - Analytical Chemistry Lab

(Any 15 experiments from category 1-9 and demonstration experiments)

1. Water analysis
   a) Estimation of total alkalinity of water
   b) Estimation of dissolved oxygen in waste water
   c) Estimation of chloride content in water
   d) Estimation of hardness in water by EDTA
   e) Chemical oxygen demand (COD)
2. Milk analysis
   a) Determination of specific gravity & acidity of milk
   b) Estimation of total solid content in milk
   c) Estimation of ash content in milk
   d) Estimation of fat content in milk
   e) Estimation of lactose content in milk
3. Butter analysis
   a) Estimation of moisture content in butter
   b) Estimation of curd & salt in butter
   c) Estimation of fat in butter
4. Drug analysis
   a) Estimation of Isoniazin by $KMnO_4$ method and bromine method
   b) Estimation of ascorbic acid in a given tablet
   c) Estimation of pot. phenoxy methyl penicillin in a given tablet
   d) Estimation of sulphanilamide
   e) Estimation of salicylic acid
5. Cement analysis
6. Estimation of caffeine from tea
7. Analysis of antacid tablet
8. Determination of nickel content in the given vanaspathi sample
9. Estimation of nickel content in steel sample

Demonstration experiments

10. Blood analysis
    a) Estimation of cholesterol in blood
    b) Estimation of glucose in blood
    c) Estimation of urea in blood
11. Urine analysis
    a) Ketone bodies in urine
    b) Albumin in urine
    c) Glucose in urine

References:

1. Manual provided by the department.
2. A. I. Vogel, Text Book of Quantitative Inorganic Analysis, 5^{th} Edn, Longman, 1989.

CH 613 - Synthetic Organic Chemistry

Introduction to retrosynthesis: Synthon, synthetic equivalent, target molecule, functional group interconversion, disconnection approach, importance of the order of events in organic synthesis. Chemoselectivity, one group C-C and C-X disconnection (disconnection of alcohols, alkenes, and carbonyl compounds).

Two group C-C & C-X disconnections: 1,3 and 1,5 difunctionalised compounds, α,β-unsaturated carbonyl compounds, control in carbonyl condensation, synthesis of 3,4,5 and 6 membered rings in organic synthesis. Diels- Alder reaction, connection in retro synthesis.

Protecting groups: Protection of hydroxyl, carboxyl, carbonyl, amino groups. Umpolung reagents, definition of umpolung, acyl anion equivalent, protection of carbon-carbon multiple bonds. Illustration of protection and deprotection in synthesis.

Reagents in organic synthesis: Functional group transformation, complex metal hydrides, Gilman's reagent, lithium diisoproplyamide (LDA), dicyclohexylcarbodimide, timethylsilyl iodide, Woodward and Provost hydroxylation, osmium tetraoxide, DDQ, SeO_2, lead tetraacetate, H_2O_2, phase transfer catalyst, crown ethers and Merrifield resin, Wilkinson's catalyst, Baker yeast.

Name reactions in organic synthesis: Peterson olefination, McMurry, Shapiro reaction, Wittig and its modifications, palladium based reactions - Suzuki, Heck, Sonagashira, Hiyama, Stille, Glazer-Eglington coupling, Sharpless epoxidation, Henry reaction, Michael addition, aldol, Claisen, Dieckman condensations, Barton, Baylis Hillman reaction, Stork enamine reaction and selective mono and di alkylation *via* enamines.

References:

1. House, Modern Synthetic Reaction, 1973.
2. S. Warren, Organic Synthesis The Disconnection approach, Wiley and sons, 2002.
3. S. Warren, Organic Synthesis The Synthon approach, 2nd Edn, Wiley and sons, 1991.

CH 615 - Solid State, Nuclear and Main Group Chemistry

Fundamentals: Types of solids - close packing of atoms and ions - bcc , fcc and hep voids - Goldschmidt radius ratio - derivation - its influence on structures - structures of rock salt - cesium chloride - wurtzite - zinc blende - rutile - fluroite - antifluorite - diamond and graphite - spinel - normal and inverse spinels and perovskite - lattice energy of ionic crystals - Madelung constant - Born-Haber cycle and its applications.

Theories: Band theory of solids. Free electron Theory, zone theory, MO theory of solids - dislocation in solids: Schottky and Frenkel defects. Line defects and plane defects – non - stoichiometric compounds. Electrical properties: Energy bands, insulators, semiconductors and conductors - super conductors - dielectric properties, piezo-electricity, ferro electricity - conductivity in pure metals. Superconductivity: Occurrence, BCS theory, high temperature super conductors - introduction to nanoparticles - metal nanoparticles - particle size determination.

X- Ray diffraction: Theory- the crystal systems and Bravais lattices - Miller indices and labelling of planes - symmetry properties - crystallographic point groups and space groups - X-ray diffraction - powder and rotating crystal methods - systematic absences and determination of lattice types - analysis of X-ray data for cubic system - structure factor and Fourier synthesis - Fundamentals of electron and neutron diffraction.

Nuclear structure: Mass and charge, nuclear moments, binding energy, mass defect, packing fraction, stability, magic numbers. Modes of radioactive decay and rate of radioactive decay - half-life, average life, radioactive equilibrium: Transient and secular - nuclear reactions: Energetics and types - nuclear fission- liquid drop model - nuclear fusion - essential features of nuclear reactors - tracer techniques, neutron activation analysis - carbon and rock dating - application of tracers in chemical analysis, reaction mechanisms, medicine and industry.

Inorganic rings and polymers: Catenation, heterocatenation, intercalation chemistry, one dimensional conductor, polymeric sulfur nitride - Preparation, properties - isopoly anions - heteropoly anions - borazines - phosphazenes - phosphazene polymers - ring compounds of sulphur and nitrogen. Interhalogen compounds - oxoacids of selenium and tellurium. Noble gas chemistry and their halides and pseudohalides.

References:

1. L.V. Azaroff, Introduction to Solids, Mc.Graw hill, New York.
2. A. R. West, Solid State Chemistry and Its Applications, John Wiley & Sons, 1984.
3. H. J. Arnikar, Essentials of Nuclear Chemistry, 4th Edn., New Age International Publishers Ltd., New Delhi, 1995.
4. F. A. Cotton, Wilkinson, G. and P. L. Gaus, Basic Inorganic Chemistry, 3rd Edn., John Wiley & Sons, New York, l995.
5. J. D. Lee, Concise Inorganic Chemistry, 5th Edn., Chapman and Hall, London, 1996.
6. J. E. Huheey, E. A. Keiter and R. L. Keiter, Inorganic Chemistry - Principles of Structure and Reactivity, 4th Edn., Harper Collins, New York, l993.

CH 617- Statistical Thermodynamics, Photochemistry and Surface Chemistry

Statistical thermodynamics I: Maxwel's law of distribution of molecular speeds, graphical representation, experimental verification - derivation of expressions for average, most probable and root mean square velocity. Concept of velocity space and phase space - perturbution and combination - laws of probability - microstates for distinguishable and indistinguishable particles. Derivation of Maxwell Boltzmann distribution law - partition functions and their calculation. Expressions for thermodynamic quantities in terms of partition functions - translational, rotational, vibrational and electronic contributions to the thermodynamic properties of perfect gases, Intermolecular forces in imperfect gases.

Statistical thermodynamics-II: Statistical interpretation of laws of thermodynamics, third law of thermodynamics and apparent expression to it. Quantum statistics: Limitation of classical statistics - quantum statistics and classical statistics, comparison - heat capacities of gases in general and hydrogen in particular - heat capacities of solids. Einstein and Debye models - Bose Einstein statistics and Fermi Dirac statistics and corresponding distribution functions - applications of quantum statistics to liquid helium, electrons in metal and Planck's radiation law.

Photochemistry: Absorption and emission of radiation, Franck Condon principle decay of electronically excited states, radiative and non-radiative processes, fluorescence and phosphorescence, spin-forbidden radiative transitions, inter conversion and intersystem crossing. Theory of energy transfer - resonance and exchange mechanism, triplet-triplet annihilation, photosensitization and quenching. Spontaneous and induced emissions. Einstein transition probability - inversion of population - laser and masers. Flash photolysis: Chemi and thermoluminescence.

Surface chemistry I: Surface Phenomena, Gibbs adsorption isotherm, types of adsorption isotherms, solid-liquid interfaces, contact angle and wetting, solid-gas interface, physisorption and chemisorption, Freundlich, derivation of Langmuir and BET isotherms, surface area determination. Kinetics of surface reactions involving adsorbed species, Langmuir-Hinshelwood mechanism, Langmuir-Rideal mechanism, Rideal-Eley mechanism.

Surface chemistry II: Surface Films, Langmuir-Blodgett films, self assembled mono layers, collapse pressure, surface area and mechanism of heterogeneous catalysis, phase transfer catalysis. Chemical analysis of surfaces: Surface preparations - spectroscopic surface characterization methods, electron spectroscopy, ion scattering spectrometry, secondary ion scattering microscopy (SIMS) - Auger electron spectroscopy - instrumentation and application. Electron stimulated micro analysis, scanning probe microscopes.

References:

1. P. W. Atkins, Physical Chemistry, 6th Edn., Oxford University Press, 1998.
2. D. McQuarie, and J. D. Simmen, Physical Chemistry, 1st Edn., University Science, 1998.
3. S. Glasstone, Thermodynamics for Chemists, Affiliated East West Press, 1965.
4. B. C. McClelland, Statistical Thermodynamics, Chapman and Hall, 1973.
5. L. K. Nash, Elements of Classical and Statistical Thermodynamics, Addison-Wesley, 1970.
6. K. K. Rohatgi - Mukkerjee, Fundamentals of Photochemistry, Wiley 1992.
7. P. K. Ghosh, Introduction to Photoelectron Spectroscopy, Wiley Interscience, 1983.

CH 619 - Fundamentals and Applications of Spectroscopy

Nuclear magnetic resonance: Concept and theory - rotating frame and laboratory frame - FT-generation and detection of FID – instrumentation - relaxation phenomena, ^{1}H- NMR - chemical shift - chemical shift anisotropy - spin-spin coupling - mechanism and sign of J coupling - AX, AB, ABC, AMX, AABB, AA′BB′ systems - Karplus relationship - second order effects - chemical shift reagents - double irradiation experiments - ^{13}C NMR –chemical shifts and line intensities

Nuclear magnetic resonance: Spin decoupling- Nuclear Overhouser effect - Solomon equations and cross relaxation - polarization transfer schemes - APT/INEPT/DEPT - dynamic processes by NMR - restricted rotation (DMF, DMA, biphenyls, annulenes), cyclohexane ring inversion, degenerate rearrangements (bullvalene and related systems), organometallic systems. Significance of coalescence temperature - analysis and applications of ^{19}F, ^{31}P, and ^{11}B spectra - other important nuclei - working of 2-D methods COSY-HETCOR - HSQC - HMQC – TOCSY – INADEQUATE - interpretation of spectra - introduction to solid state NMR - cross polarization – WAHUHA - imaging methods in magnetic resonance.

Electron paramagnetic resonance: Basic principles - hyperfine interaction - zero-field energy levels - McConnal equations – anisotropy - CW ENDOR and TRIPLE-basic principles - application to organic radicals and transition metal complexes - zero field splitting - Pulse EPR basics - model system for pulse EPR experiments - pulse schemes and applications - nuclear modulation experiments – ESEEM – HYSCORE - Davies and Mims ENDOR - distance measurements using ELDOR.

Mass spectroscopy: Methods of desorption and ionization (EI, CI, ESI, MALDI, FAB, TOF) – instrumentation - magnetic sector analysis - quadrupole analyzer - ion cyclotron resonance (FT) - determination of molecular formula - meta stable ions - study of fragmentation pattern - α-bond cleavage - McLafferty rearrangement - retro Alder fragmentation - applications in organic chemistry - isotope distribution analysis.

Mössbauer spectroscopy: Principles and applications-Hyperfine- Magnetic Interactions - NQR spectroscopy – Principles and Applications- Applications of combined spectroscopic techniques - double bond equivalence - case studies and structural identification of organic compounds and inorganic compounds

References:

1. R. S. Macomber, A Complete Introduction to Modern NMR Spectroscopy, John Wiley & Sons Ltd, 1998.
2. D. L. Pavia, G. M. Lampman, G. S. Kriz, J. A. Vyvyan, Introduction to Spectroscopy, 5th Edn., Brooks Cole , 2010.
3. J. A. Weil, J. R. Bolton, Electron Paramagnetic Resonance, Elementary Theory and Practical Applications, Wiely-Interscience, 2007.
4. A. Schweigher, G. Jeshcke, Principles of Pulse Electron Paramagnetic Resonance, Oxford University press, 2002.
5. L. D. Field, S. Sternhell, J. R. Kalman, Organic Structures from Spectra, John Wiley & Sons, Ltd, 4th and 5th Edn. 2007 & 2013.
6. M. Balci, Basic ^{1}H- and ^{13}C-NMR Spectroscopy, Elsevier, 2005.
7. J. H. Simpson, Organic Structure Determination using 2D-NMR Spectroscopy, Academic Press, 2008.

8. D. P. E. Dickson, F. J. Berry, Ed. Mossbauer Spectroscopy, Cambridge University Press, 1986.
9. M. H. Levitt, Spin Dynamics- Basics of Nuclear Magnetic Resonance, 2nd Edn, John Wiley and sons, 2008.
10. E. Breitmaier, Structure Elucidation by NMR in Organic Chemistry - A Practical Guide, 3rd Edn, John Wiley and Sons, 2002.
11. W. Hendreson, J. S. McIndoe, Mass Spectrometry of Inorganic, Coordination and Organometallic Compounds, John Wiley and Sons, 2005.
12. K. Nakamoto, Infrared and Raman Spectra of Inorganic and Coordination Compounds Part A &Part B, 2nd Edn, Wiely, 2009.
13. A. B. P. Lever, Inorganic Electronic Spectroscopy, 2nd Edn, Elsevier, 1984.

CH 621 - Inorganic and Organic Quantitative Analysis Lab

Inorganic quantitative analysis

Analysis involving volumetric and gravimetric estimations of mixtures of cations Cu & Ni; Cu & Zn; Zn & Cu; Fe & Ni; Fe(II) & Fe(III)

Organic quantitative analysis

(a) Estimations:

Estimation of phenol, aniline, ascorbic acid.
Estimation of ketone by volumetric method & gravimetric method.
Estimation of lactose in milk.
Estimation of glucose by Fehlings method.
Estimation of glucose by Bertrand's method.

(b) Analysis of oils:

Determination of saponification value of an oil, Determination of acetyl value of an oil, Determination of iodine value of an oil, Determination of acid value of an oil.

References:

1. A. I. Vogel, Text Book of Quantitative Inorganic Analysis, 5th Edn, Longman, 1989
2. A. I. Vogel, 'Text book of Practical Organic Chemistry',5th Edn. ELBS, London, l989.
3. B. B. Dey and M. V. Sitharaman, 'Laboratory Manual of Organic Chemistry' Revised by T.R. Govindachari, Allied Publishers Ltd., New Delhi. 4th Revised Edn., l992.

CH 623 - Computational and Spectroscopy Lab

Computational Chemistry Lab. Experiments

1. Curve fitting for Beer Lamberts law
2. Normalized radial wave function for 1s atomic orbital of hydrogen atom
3. Radial distribution function for 1s atomic orbital
4. Simulation of potentiometric titration plots
5. Computation of energy gap based on particle in 1D models, plot of its wave function and probability density
6. Single point energy of water - comparison based on equipartition principle and quantum principles
7. Single point energy of formaldehyde, visualization of molecular orbitals
8. Evaluation of NMR properties of butane, trans 2-butene and 2-butyne
9. Geometry optimization of ethylene and comparison with fluoro ethylene
10. Geometry optimization and MO energy of ethylene, butadiene and hexatriene, crotonaldehyde - types of electronic transitions, transition dipole evaluation

Spectroscopy

1. Fabry Pyrot Etalon - Spacing of Etalon-Finesse and free spectral range
2. Zeeman effect - Analysis of Planks constant and Bohr magneton
3. Michelson's interferometer - Wavelength of laser, refractive index, magneto strictive properties of ferromagnetic materials
4. Calculation of extinction coefficient
5. Diffraction gratings - Wavelength of light
6. Photoelectric effect- Planks constant - Work function of material
7. Fluorescence spectroscopy - Excitation and emission, Kashas rule
8. Absorption spectroscopy - Beers law – Deviations - Titrations
9. Polarization of light - Rayleigh scattering - Dichorism and birefringence
10. Spin Evolution Demo and Spectral Simulation and Fitting

References: Manual provided by the department.

CH 625 - Catalysis

Fundamentals: Catalyst - activation energy concept - types of catalysis - comparison of homogeneous & heterogeneous catalysis - enzyme catalysis - green catalysis - nano catalysis - autocatalysis - phase transfer catalysis - promoters - poisons - examples.

Homogeneous catalysis: Noyori asymmetric hydrogenation - metal mediated C-C and C-X coupling reactions - Heck, Stille, Suzuki, Negishi and Sonogashira, Nozaki-Hiyama, Buchwald-Hartwig, Ullmann coupling reactions - directed ortho metalation - metal (Rh, Ir) catalyzed C-H activation reactions and their synthetic utility - copper and rhodium based carbene and nitrene complexes - cyclopropanation - Rh catalyzed C-H insertion and aziridination reactions including asymmetric version - introduction to N-heterocyclic carbene metal complexes.

Characterization of solid catalysts: Surface area - structure - surface morphology - porosity - pore volume - diameter - particle size - X-ray diffraction - SEM, TEM, X-ray absorption spectroscopy, XPS and Auger spectroscopy to surface studies - TPD, TPR for acidity and basicity of the catalysts - theories - boundary layer theory - Wolkenstein theory - Balanding's approach.

Heterogeneous catalysis: Adsorption isotherms - surface area - pore size and acid strength measurements - porous solids - catalysis by metals - semiconductors and solid acids - supported metal catalysts - catalyst preparation - deactivation and regeneration - model catalysts - ammonia synthesis - hydrogenation of carbon monoxide - hydrocarbon conversion - selective catalytic reduction - polymerization.

Photocatalysis: Porphyrins - phthalocyanines and semiconductor as photo catalysts in photolysis reactions - generation of hydrogen by photo catalysts - photo catalytic break down of water and harnessing solar energy - photocatalytic degradation of dyes - environmental applications.

References:

1. P.H. Emmet, Catalysis (Vol I and II), Reinhold, New York, 1954.
2. M. Schlosser, Organometallics in Synthesis, A manual, John Wiley, New York, 1996.
3. L.S. Hegedus, Transition Metals in the Synthesis of Complex Organic Molecules, University Science, Book, CA, 1999.
4. D.K. Chakrabarty and B. Viswanathan, Heterogeneous Catalysis, New Age, 2008.
5. B. Viswanathan, S. Kannan, R.C. Deka, Catalysts and Surfaces: Characterization Techniques, Narosa, New Delhi, 2010.
6. M. Kaneko, I. Okura, Photocatalysis: Science and Technology, Springer, 2003.

CH 627 - Environmental Chemistry

Scope: Environmental pollution - structure of atmosphere - biogeological cycles - oxygen - nitrogen – carbon – phosphorous – sulphur - biodistribution of elements - air pollutions - reactions in atmosphere - primary pollutants - air quality standards - analysis of CO, nitrogen oxides, sulphur oxides, hydrocarbons and particulate matter - particulate pollution - control methods - vechicular pollution - green house effect and global warming - climatic changes – ozone - photochemical smog - acid rain - sampling - monitoring – control.

Hydrosphere: Water pollution - hyrological cycle - chemical composition - sea water composition - water quality criteria for domestic and industrial uses - BIS and WHO standards - ground water pollution - surface water pollution - lake and river water - eutrophication - marine pollution - water pollutants - biodgradeability of detergents – pestisides - endosulfan and related case studies.

Classification of industrial waste waters: Principles of water and waste water treatment - aerobic and anaerobic treatment - industrial waste water treatment - heavy metal pollution - hard water - softening - purification of water for drinking purposes - water treatment for industrial use - electrodialysis - reverse osmosis - other purification methods - chemical speciation of elements.

Water analysis: Color - odor - conductivity - TDS - pH - acidity - alkalinity - chloride - residual chlorine - hardness - trace metal analysis - elemental analysis - ammonia - nitrite - nitrate - fluoride - sulphide - phosphate - phenols - surfactants - BOD - COD - DO - TOC - nondispersive IR spectroscopy - anode stripping - ICP - AES - Chromatography - ion selective electrodes - neutron activation analysis.

Soil pollution: Soil humus - soil fertility - inorganic and organic components in soil - acid - base and ion exchange reactions in soils - micro and macro nutrients - wastes and pollutants in soil - introduction to geochemistry - solid waste management - treatment and recycling- soil analysis - radioactive pollution - disposal of radioactive waste.

References:

1. H. Kaur, Environmental Chemistry, 6th Edn, Pragathi Prakashan, Meerut, 2011.
2. K.H.Mancy and W,.J.Weber Jr. Wiley, Analysis of Industrial Waste Water, Interescience New York, 1971.
3. L.W. Moore and E. A. Moore, Environmental Chemistry, McGraw Hill Publication, New York, 2002.
4. S. M. Khopkar, Environmental Pollution Analysis, New Age International (P) Ltd, 1993.
5. Colid Baird. Environmental Chemistry, W. H. Freemand and Company, 1995.

CH 629 -Inorganic Rings, Cages and Clusters

Main group clusters: Geometric and electronic structure, three - four and higher connect clusters, the closo-, nido-, arachno- borane structural paradigm, Wade-Mingos and Jemmis electron counting rules, clusters with nuclearity 4-12 and beyond 12. Structure, synthesis and reactivity.

Transition metal clusters: Low nuclearity metal carbonyl clusters and 14n+2 rule, high nuclearity metal carbonyl clusters with internal atoms, structure, synthesis and reactivity - capping rules.

Isolobal analogy: Heteronuclear clusters - carboranes and heteroboranes - metal clusters - structural prediction of organometallic clusters - main group transition metal clusters: Isolobal analogs of p-block and d-block clusters - interstitial systems - cubanes and zintl clusters.

Inorganic homo- & heterocycles: Synthesis, structure and reactivity - structural variety & properties of borazins and phosphazenes, borides, carbides, silicides, nitrides, phosphides, oxides and sulphides of transition elements, multiple bonds and cluster variety of transition metals.

Inorganic rings and polymers: Definition, variety and merits, P, Si, S, N, & O based polymers, poly-phosphazenes, poly-thiazenes, poly-siloxanes and poly-silanes.

References:

1. D. M. P. Mingos and D. J. Wales, Introduction to Cluster Chemistry, Prentice Hall, 1990.
2. N. N. Greenwood and E. A. Earnshaw, Chemistry of Elements, Pergaman Press, 1984.
3. I. Haiduc & D. B. Sowerby (Eds.), Inorganic Homo-and Heterocycles Vols. 1 & 2, Academic Press, 1987.
4. J. E. Mark, R. West & H. R. Allcock, Inorganic Polymers, Academic Press, 1992.
5. T. P. Fehlner, J. F. Halet and J-Y. Saillard, Molecular Clusters: A Bridge to Solid-State Chemistry, Cambridge University Press, 2007.
6. P. Braunstein, L. A. Oro, P. R. Raithby, Ed. Metal Clusters in Chemistry, John Wiley and sons, 1999.
7. T. Chivers, I. Manners, Inorganic Rings and Polymers of the p-Block Elements, from Fundamentals to Applications, RSC Publishing, 2009.

CH 631 - Medicinal Chemistry

Introduction: History of medicinal chemistry, general mechanism of drug action on lipids, carbohydrates, proteins and nuleic acids, drug metabolism and inactivation, receptor structure and sites, drug discovery development, design and delivery systems, gene therapy and drug resistance.

Classification: Drugs based on structure or pharmacological basis with examples, synthesis of important drugs such as α - methyl dopa, chloramphenicol griseofulvin, cephelosphorins and nystatin. Molecular modeling, conformational analysis, qualitative and quantitative structure activity relationships.

General introduction to antibiotics: Mechanism of action of lactam antibiotics and non lactam anti biotics, antiviral agents, chemistry, stereochemistry, biosynthesis and degradation of penicillins - An account of semisynthetic penicillins - acid resistant, penicillinase resistant and broad spectrum semisynthetic penicillins.

Elucidation of enzyme structure: Mechanism, kinetic, spectroscopic, isotopic and stereochemical studies. Chemical models and mimics for enzymes, design, synthesis and evaluation of enzyme inhibitors.

Interactions: DNA-protein interaction and DNA-drug interaction. Introduction to rational approach to drug design, physical and chemical factors associated with biological activities, mechanism of drug action.

References:

1. I. Wilson, Giswald and F. Doerge, Text Book of Organic Medicinal and Pharmaceutical Chemistry, J.B. Lippincott Company, Philadelphia, 1971.
2. A. Burger, Medicinal Chemistry, Wiley Interscience, New York, Vol. I and II, 1970.
3. Bentley and Driver's Text Book of Pharmaceutical Chemistry revised by L.M. Artherden, Oxford University Press, London, 1977.
4. A. Gringauz, Introduction to Medicinal Chemistry, How Drugs Act and Why?, John Wiley and Sons, 1997.
5. G. L. Patrick, Introduction to Medicinal Chemistry, Oxford Univeristy Press, 2001.

CH 633 - Nano Science and Technology

Introduction to nanoscience and nanotechnology: Underlying physical principles of nanotechnology: *Nanostructured Materials: Size is Everything.* - fundamental physicochemical principles - size dependence of the properties of nanostructured matter - quantum confinement, single electron charging, the central importance of nanoscale morphology. Societal aspects of nanotechnology: Health, environment, hype and reality.

The advent of the nanomaterial. Top down and bottom up approaches to building materials. Properties of nanomaterials such as nanoparticles, carbon nanotubes. Overview of self-assembly. Inert gas condensation, arc discharge, RF plasma, plasma arc technique, ion sputtering, laser ablation, laser pyrolysis, ball milling, molecular beam epitaxy, chemical vapour deposition method and electro deposition.

The basic tools of nanotechnology: Scanning electron microscopy (SEM), TEM and EDAX analysis and X-ray diffraction, A brief historical overview of atomic force microscopy (AFM) and an introduction to its basic principles & applications. Optical microscope and their description, operational principle and application for analysis of nanomaterials, UV-VIS-IR spectrophotometers, Principle of operation and application for band gap measurement.

Metal nanoparticles: Size control of metal nanoparticles and their characterization, study of their properties, optical, electronic, magnetic. Surface plasmon band and its applications, role in catalysis, alloy nanoparticles, stabilization in sol, glass, and other media, change of band gap, blue shift, colour change in sol, glass, and composites, plasmon resonance.

Carbon nano structures: Introduction. Fullerenes, C60, C80 and C240 nanostructures. Properties & applications (mechanical, optical and electrical). Functionalization of carbon nanotubes, reactivity of carbon nanotubes. Nanosensors: Temperature sensors, smoke sensors, sensors for aerospace and defense. Accelerometer, pressure sensor, night vision system, nano tweezers, nano-cutting tools, integration of sensor with actuators and electronic circuitry biosensors.

References:

1. T. Pradeep, Nano: The Essentials, Tata McGraw-Hill, New Delhi, 2007.
2. G. Cao, Nanostructures and Nanomaterials – Synthesis, Properties and Applications, Imperial College Press, London, 2004, chapters 3, 4 and 5.
3. C. N. R.Rao, A. Muller and A. K. Cheetham, The Chemistry of Nanomaterials, Volume 1, Wiley –VCH Verlag GmbH & Co. KgaA, Weinheim, 2004, Chapter 4.

CH 635 - Nuclear Chemistry

Discovery: Types of decay - decay kinetics: decay constant, half-life period, mean life parent - daughter decay - growth relationships - secular and transient equilibrium - units of radioactivity - alpha, beta and gamma decay: Theory of decay, energies and properties - artificial radioactivity - detectors: Ionization chamber, electron pulse counters, scintillation detectors, semiconductor, detectors, thermo luminescence detectors and neutron detectors.

Types of nuclear reactions: Bethe notation, the compound nucleus theory - reaction cross – section - transmutation reactions, elastic and inelastic scattering, spallation, fragmentation, stripping and pick-up, fission, fusion, photonuclear reactions, thermonuclear reactions.

The fission energy - reproduction factor - classification of reactors - based on moderators, coolent, phase of fuel and generation - principle of thermal nuclear reactors. The four factor formula - reactor power - critical size of a thermal reactor - excess reactivity and control - breeder reactor - reprocessing of spent fuels - nuclear waste management - safety culture - active and passive safety, containment building, nuclear criticality safety, ionizing radiation protection - enforcement agencies.

Radiation chemistry: Passage of radiation through matter - units for measuring radiation absorption - radiation dosimetry - radiolysis of water - free radicals in water radiolysis - chemical dosimetry: Radiolysis of Fricke dosimeter solution - radiation - induced color centers in crystals - Effects of radiation with matter: Radiolysis of inorganic gases, organic gases, organic compounds, solids, and polymers - Annealing of radiation damage.

Application of radioisotopes: Probing by isotopes, reactions involved in the preparation of radioisotopes, the Szilard-Chalmer's reaction - radiochemical principles in the use of tracers - applications of radioisotopes as tracers - chemical investigations, analytical applications, agricultural and industrial applications - neutron activation analysis - carbon and rock dating - use of nuclear reactions - radioisotopes as source of electricity - nuclear medicines.

References:

1. W. Loveland, D. Morrissey, G. Seaborg. Modern Nuclear Chemistry, Wiley-Interscience, Hoboken, NJ, 2006.
2. Arnikar, H. J., Essentials of Nuclear Chemistry, 4th Edn., New Age International Publishers Ltd., New Delhi, 1995.
3. K. H. Lieser, Nuclear and Radiochemistry, 2nd revised ed., Wiley-VCH, Berlin, 2001.
4. G. Choppin, J. O Liljenzin and J. Rydberg. Radiochemistry and Nuclear Chemistry. 3rd ed. Butterworth-Heinemann, Oxford, 2002.
5. G Friedlander, GW Kennedy, ES Macias and JM Miller. Nuclear and Radiochemistry. 3rd ed., John Wiley & Sons, New York, 1981.
6. S. Glasstone, Source Book on Atomic Energy, Krieger Pub Co, 3rd Edn, 1979.

CH 616 - Computational Methods in Chemistry

C - Syntax: Character set - constants and variables, data types and sizes, declarations, operators - expressions - conditional expressions, precedence and order of evaluation, statements and blocks, if-else, if-else-if and switch statements, while, for and Do - while loops, break and continue statements, Go to and labels, basics of functions and types, header files, recursion, arrays – 1D and 2D, file handling concepts.

Kinetics - solving rate equations, thermodynamics - heats of reactions, heat capacity, entropy, spectroscopy - moment of inertia, wave numbers of stokes and anti-stokes Raman lines, masses of isotopes from rotational and vibrational spectroscopic data - Group theory - Huckel MO calculations of delocalisation energy, hybridisation schemes and symmetries of vibrations in non - linear molecules. Crystallography - d spacings for an orthorhombic crystal, Fourier synthesis of electron density using structure factor, axial angles of a triclinic crystal.

Solving polynomial equations - Newton - Raphson method, solutions of simultaneous equations - Gauss elimination, Jacobi iteration and matrix diagonalisation, numerical differentiation and integration - Simpson's rule, trapezoidal rule - determination of entropy, solution of differential equations - Runge-Kutta method - theory and application to thermodynamics, linear and non-linear curve fitting.

Force field methods - force field energy and parameterization, electronic structure methods - SCF techniques, semi-empirical methods, basis sets and their classification, density functional theory and methods.

Geometry convergence, energy convergence, dipole moment convergence, vibrational frequencies convergence, bond dissociation curve, angle bending curve, transition state modeling using Chemoffice and Gaussian software - demo on docking software.

References:

1. K. V. Raman, Computers in Chemistry, Tata McGraw Hill, 1993.
2. F. Jensen, Introduction to Computational Chemistry, John Wiley & Sons, 2003.
3. C. Balagurusamy, Programing in C, Tata McGraw Hill, 1997.
4. M. K. Jain, Numerical Methods for Scientific and Engineering Computation, Wiley Eastern Ltd, 1995.
5. User manuals of Gaussian09, Chemoffice Ultra and Gauss View.

CH 618 - Natural Products Chemistry

Classification of natural products: Chemical structure, classification, structure elucidation based on degradative reactions. Isolation and structural elucidation of selected alkaloids and terpenes - quinine, morphine, and reserpine, citral, juvabione and logifolene.

Amino acids: Synthesis of amino acids - reactions – properties - amino acids in nature: β-amino acids and their metabolites in nature - structure of proteins - peptides, insect pheromones.

Steroids: Classification - synthesis and structure elucidation of cholesterol, conversion of cholesterol to progesterone - androsterone and testosterone - cortisone - vitamin D.

Nucleic acids: Structure of nucleosides and nucleotides - RNA and DNA, complimentary base pairing - Watson and Crick model. DNA-drug interaction.

Carbohydrates: Determination of configuration - Hudsons rules - structure of sugars - transformation of sugers, preparation of alditols, glycosides, deoxysugars. Synthesis of vitamin C from glucose.

References:

1. I. L. Finar, Organic Chemistry Vol. I & Vol. II- Pearson Education, 6th edn.
2. F. A. Carey and R. J. Sundberg, (Eds) 3rd Edition, Part B. Plenum/Rosetta, 1990.
3. I. Fleming, Selected Organic Synthesis, John Wiley and sons, 1982.
4. Atta-ur-Rahman, Studies in Natural Products Chemistry, Vol.1 and 2, Elsevier, 1988.
5. R. Krishnaswamy, Chemistry of Natural Products; A Unified Approach, Universities Press.
6. R. J. Simmonds: Chemistry of Biomolecules: An Introduction, RSC.

CH 620 - Polymer Chemistry

Concept of macromolecules: Principle of duality and molecular design - tetrahedral model of product development. Nomenclature and classification. Raw material for the synthesis of polymers. Synthetic schemes. Petroleum and petrochemicals - Naphtha as a source of petrochemicals.

Polymerization processes: Free radical addition polymerization - kinetics and mechanism. Chain transfer. Molecular weight distribution and molecular weight control. Cationic and anionic polymerization: Kinetics and mechanism. Living polymers. Step growth polymerization - Linear *Vs* cyclic polymerization. Other methods of polymerization - bulk, solution, melt, suspension, emulsion and dispersion techniques.

Polymer stereochemistry: Configuration and conformation. Tacticity. Chiral polymers. Polymer characterization. Molecular weights - Methods for determining molecular weights - static, dynamic, viscometry, light scattering and GPC. Crystalline and amorphous states. glassy and rubbery States. Glass transition temperature and crystalline melting of polymers. Degree of crystallinity - X-ray diffraction. Thermal stability of polymers.

Polymer solutions: Flory-Huggins theory. Chain dimension - chain stiffness. End-to-end chain distance of polymers. Conformation - random coil, solvation and swelling. Determination of degree of cross linking and molecular weight between cross links. Industrial polymers - synthesis, structure and applications of industrially important polymers.

Specialty polymers: Polymers as aids in organic synthesis. Polymeric reagents, catalysts, substrates. Liquid crystalline polymers - Main chain and side chain liquid crystalline polymers. Phase morphology. Conducting polymers - Synthesis & applications of polyacetylenes, polyanilines, polypyrroles & polythiophines. Photoresponsive and photorefractive polymers. Polymers in optical lithography - Drug delivery - Drug carriers - Polymer based nanoparticles.

References:

1. F.W. Billmayer. Textbook of Polymer Science. 3rd Edn, Wiley. N.Y. 1991.
2. J.M.G Cowie. Polymers: Physics and Chemistry of Modern Materials. Blackie. London, 1992.
3. R.J.Young, Principles of Polymer Science, 3rd Edn. , Chapman and Hall. N.Y. 1991.
4. P.J. Flory. A Text Book of Polymer Science. Cornell University Press. Ithacka, 1953.
5. F. Ullrich, Industrial Polymers, Kluwer, N.Y. 1993.
6. H.G.Elias, Macromolecules, Vol. I & II, Academic, N.Y. 1991.
7. J.A.Brydson, Polymer chemistry of Plastics and Rubbers, ILIFFE Books Ltd., London, 1966.