MASTER OF SCIENCE IN CHEMISTRY

SYLLABUS FOR THE
CREDIT BASED CURRICULUM

FROM 2011 ONWARDS

Department of Chemistry
National Institute of Technology
Tiruchirappalli – 620 015

M. Sc. Chemistry 2011 onwards

Code	Course	L	T	P	C
Semester 1					
CH 601	Organic Chemistry: Reaction Mechanisms and Their Types	3	-	-	3
CH 603	Coordination Chemistry: Bonding, Spectra and Reactions	3	-	-	3
CH 605	Quantum Chemistry and Group Theory	3	-	-	3
CH 607	Analytical and Instrumental Methods in Chemistry	3	-	-	3
CH 609	Organic Chemistry Practicals	-	-	6	2
CH 611	Analytical Chemistry Practicals	-	-	6	2
					16
Semester 2					
CH 602	Photochemistry and Pericyclic Reactions	3	-	-	3
CH 604	Organometallic Chemistry	3	-	-	3
CH 606	Bio Inorganic Chemistry	3	-	-	3
CH 608	Thermodynamics, Electrochemistry and Kinetics	3	-	-	3
CH 610	Inorganic Chemistry Practicals	-	-	6	2
CH 612	Physical Chemistry Practicals	-	-	6	2
					16
Semester 3					
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	Spectroscopy	3	-	-	3
CH 621	Comprehensive Viva voce	3	-	-	3
CH 623	Seminar: Review of Literature and Methodology	-	-	-	3
					18
Semester 4					
CH 614	M. Sc. Project and Viva voce	-	-	-	8
	ELECTIVE I	3	-	-	3
	ELECTIVE II	3	-	-	3
	ELECTIVE III	3	-	-	3
CH 616	Biochemistry	CH 618	Catalysis		
CH 620	Computational Chemistry	CH 622	Electron Spectroscopy		
CH 624	Environmental Chemistry	CH 626	Medicinal Chemistry		
CH 628	Nano Science and Technology	CH 630	Natural Products Chemistry		
CH 632	Novel Inorganic Compounds	CH 634	Nuclear Chemistry		
CH 636	Polymer Chemistry				
					17
Total minimum credits required					**67**

Semester 1

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.

Aliphatic Nucleophilic Substitution– reactivity, structural and solvent effects, substitution in S_N1, S_N2, S_Ni. Neighboring 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 hof mann, 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.

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

Text Books:

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

References:

1. Peter Sykes, A guide book to mechanism in Organic chemistry, Orient-Longmens, 6th Edn, 1996.
2. E. J. Eliel, Stereochemistry of Carbon Compounds, John Wiley, 1997
3. P. Y. Bruice, Organic Chemistry. Pearson Education, 3rd edition, 2006

CH 603 – Coordination Chemistry: Bonding, Spectra and Reactions

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.

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 – electronic spectra of $[Ru(bpy)_3]^{2+}$ - 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: in the 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 - resonance Raman spectroscopy,

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 fields 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.

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

Text Books:

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 Editions, 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, "Moden Coordination Chemistry", Inter Science Publisher, 1960.

References:

1. B. E. Douglas, H. Darl , McDaniel and J. J. Alexander, Concepts and Models of Inorganic Chemistry, John Wiley &Sons, Inc. 3rd Edn, New York, l994.

2. D. F. Shriver, P. W. Atkins and C. H. Langford, 'Inorganic Chemistry', Oxford University Press, Oxford, l994.
3. K. Nakamoto, Infrared and Raman Spectra of Inorganic and Coordination Compounds Part A &Part B, 2nd Edn, Wiely. 2009

CH 605 - Quantum Chemistry and Group Theory

Quantum Chemistry-I: The Failures of Classical Physics – Block 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, and MO treatment of H-bonded systems, ethylene, butadiene and benzene. Approximation methods; Perturbation and variation method, wave functions for many electron atoms –Hartres – 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.

Text Books:

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.

References:

1. D. A. McQuarrie, 'Quantum Chemistry', University Science Books, 1983.
2. F. A. Cotton, 'Chemical Applications of Group Theory', 2nd Edn., Wiley Eastern Ltd., 1990.
3. R. K. Prasad, Quantum Chemistry, TMH, 1995
4. P.W. Atkins, 'Physical Chemistry', 6th Edn., Oxford University Press, 1998.

CH 607- Analytical and Instrumental Methods in Chemistry

Separation Techniques: Solvent extraction methods -super critical fluids- Electrophoresis: theory and applications- Chromatography- Concepts-retention parameters and selectivity- HPLC-theory and instrumentation - Ion exchange-Gel Permeation - Gas chromatography – basic instrumental set up-carriers- columns- different detectors TCD, FID, ECD and NPD- CHN analysis by GC- other elemental analysis methods

Electroanalytical methods: Electrogravimetry- Coulometry- applications- Ion-Selective electrodes- immobilized enzyme electrodes and molecular selective electrodes-Polarography – current – voltage curve. Stripping voltammetry, DME- Construction-Half-wave potential-Instrumentation-Applications of Polarography. Pulse and differential pulse polarography-Voltammetry, Excitation signals in voltammetry, Amperometric titrations – Applications. Cyclic voltammetry-Theory and applications.

Atomic Spectra: Flame Emission and Atomic Absorption Spectrometer- Instrumentation of AAS- the flame spectra, flame characteristics- Atomizers used in spectroscopy- Hollow cathode lamp- interference in AAS-applications- Atomic Emission Spectroscopy- DCP and ICP-MS-simultaneous multi element analysis.

Instrumentation basics: Elementary electronics- semiconductors- semiconductor diodes-transistors-mechanism of amplification- field effect transistors – transformers- rectifiers- voltage regulators-noise-signal-to –noise ratio- readout devices- cathode ray tube- Basic Instrumentation-Sources- monochromators- Sampling and transducers- single beam and double beam instruments- UV- Vis Instrumentation- IR sources and Transducers -Michelson interferometer - Beer-Lambert Law, Deviations, Applications- Photometric Titrations- Nephelometry and Turbidimetry

Thermal methods of Analysis: TG, DTA and DSC - Instrumentation and Theory. TG of copper sulfate pentahydrate and calcium oxalate monohydrate. Calculations of thermodynamic parameters. Labeling methods- Radio Immuno assays- ELISA test-immuno fluorescence-neutron activation analysis

Text Books:

1. G. H. Geeffery etal., 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

References:

1. F. Rouessac and A. Rouessac, Chemical Analysis: Modern Instrumentation Methods and Techniques, 2nd edn, John Wiely and Sons
2. D. A. Skoog, E. J. Holler, S. R. Crouch , Principles of Instrumental Analysis, 6th edition, Thomson Brooks Cole , 2007
3. F. W. Fifield and D. Kealey, Principles and Practice of Analytical Chemistry, 2nd Edition, International Book Company, London, 1983
4. 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 Chemistry Practicals

(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.

(c) Drug Analysis

Estimation of Isoniazin by $KMnO_4$ method and bromine method.

Estimation of Ascorbic acid in a given tablet., Estimation of pot. phenoxy methyl penicillin in a given tablet.

(d) 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-nitroniline 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.,

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(e) Extraction: Extraction of caffeine from tea leaves.

(f) Chromatography: i. Separation of Anthocyanidine from Hibiscus Rosasinens., ii. Separation of sugars.iii. Separation of Amino Acids.

Separation and characterization of two component and three component mixtures.

Text Books:

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 – Analytical Chemistry Practicals

Determination of Copper, Iron, Ca and Mg in a mixture (EDTA)
Magnesium, manganese and zinc in a mixture (fluoride masking EDTA)
Kinetic Masking Chromium and Iron in a mixture
Redox tirtations
Solvent extraction: Determination of Boron using Ferroion
Estimation of magnesium in antacid tablets.
Estimation of available Chlorine in Bleaching powder
Estimation of Na_2CO_3 in NaOH, % purity of Washing soda
Estimation of dissolved oxygen in different water samples
Estimation of Molecular mass of Organic Acids
Water Analysis (TDS, Alkalinity, Hardness, COD, DO and Chloride)
Uv-Vis and Photometric estimation of metal ions
Estimations of metal ions in real samples using AAS
Estimation of Phosphate by Nephelometry.
Analysis of a mixture by Gas Chromatography.
Determination of N,P and K in a fertilizer sample
Identification and Quantification of a drug using HPLC

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

Semester 2

CH 602-Photochemistry and pericyclic 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.

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.

Theories of Aromaticity and 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. Aliphatic electrophilic substitution SE1, SE2, SEi mechanisms.

Text Books:

1. House, Modern Synthetic Reactions, 1973.

References:

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

CH 604 - Organometallic Chemistry

Structure and Bonding in Organometallics- 18-electron rule- Metal Carbonyls-Bonding-spectra- Nitrosyls-dinitrogen complexes-Phosphines- Metal Alkyls, Aryls, Hydrides and dihydrogen complexes- π- Bound Ligands- Fluxional Molecules-Physical methods in organometallics

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- Asymmetric 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. C-H and C-C activation- Agostic Bonds - Alkene Metathesis-Mechanism- ROMP, SHOP and ADMET- C-H bond Activation-Ziegler-Natta Polymerization of olefins-Telomerization

Other Reactions: Heck Reaction- The Pauson Khand reaction- Ene reaction, Susuki coupling-Dotz reaction -Vollhardt reaction-Murai reaction-Stille Coupling- Sonagashira coupling-Alkene carbometalation- The Hartwig-Buchwald Amination- Metallocenes-Electronic Structure and Bonding in Ferrocene- Synthesis, Physical and Spectroscopic properties of metallocenes

Inorganic Cages and Clusters- Isolobal Analogy- Metal clusters-structure and bonding of boron hydrides- carboranes and heteroboranes - metal clusters - structural prediction of organometallic clusters- Spectral and magnetic properties of lanthanide and actinide complexes - Chemical Shift reagents

Text Books:

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. J. E. Huheey, E. A. Keiter and R. L. Keiter "Inorganic Chemistry, Principles of Structure and Reactivity", 4th Edition, Harper Collin College Publishers, 1993

References:

1. J. P. Collman, Principles and Applications of Organotransition Metal Chemistry, Standford University
2. Susan E. Kegley and Allan R. Pinhas, Problems and Solutions in Organometallic Chemistry, University Science Books
3. C. Elschenbroich, Organometallics, 3rd Edn, Wiely VCH
4. M. Bochmann, Organometallics 1&2 , Oxford university press, 1994

CH 606 - Bioinorganic Chemistry

Scope of Bioinorganic Chemistry: Inorganic elements in biological systems- cells- biological ligands- amino acids-proteins-nucleotides, carbohydrates and lipids- basic bioenergetics, classification of enzymes- Biochemistry: Distribution, biological roles- enzyme stabilization - blood clotting and biological calcification

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 transferrin- Storage of iron by ferritin- bio chemistry of calcium as hormonal messenger.

Metalloporphyrins: Structure and optical spectra; heme proteins- magnetic susceptibility, epr and electronic spectra- Dioxygen transport and storage-hemoglobin and myoglobin: molecular structures, thermodynamics and kinetics of oxygenation- 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

Metalloenzymes: Copper enzymes- superoxide dismutase- ceruloplasmin- Coenzymes- Molybdenum enzyme- xanthine oxidase- Zinc enzymes- carbonic anhydrase, carboxy peptidase- and interchangeability of zinc and cobalt in enzymes- Vitamin B12 and B12 coenzymes-

Photosynthesis- Photosystem-I & II (Mn(IV))- Metallothioneins- nitrogen fixation-biochemistry of iron.

Metals in Medicine: Beneficial, essential, and toxic elements-Metal deficiency and disease-toxicity of mercury, cadmium, lead, beryllium, selenium and arsenic- biological defense mechanisms- chelation therapy- metals used for diagnosis and chemotherapy- platinum complexes as anticancer drugs, Pt-DNA binding, complexes of gold, copper- zinc, mercury, arsenic and antimony as drugs-Bioorganometallic Chemsitry

Text Books

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

Reference Books

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

CH 608-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, determination, 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 overpotential –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 is parameters.

Text Books:

1. S. Glasstone, Thermodynamics for chemists, Affiliated East West Press, 1965.
2. Atkins, P.W. 'Physical Chemistry', 6th Edn., Oxford University Press, 1998.

References:

1. K, J. Laider, 'Chemical Kinetics', 3rd Edn., Harper and Row Publishers, 1987.
2. J. O. M. Bockris and A. K. N. Reddy, Modern Electrochemistry, Plenum Press, 1970.
3. J. Rajaram and J. C. Kuriacose, Thermodynamics for Students of Chemistry, Shobanlal Nagin Chand Co, 1986

CH 610- Inorganic Chemistry Practicals

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 four Compounds:
Pottassium Trioxalato Cobaltate
Bromopentammino Cobalti Chloride
Tris Ethylenediammine Chromium (III)Chloride
HexammineCobalt(III)chloride
Trisethylenediamminecobalt(III)chloride
Cis and Trans Dichlorobisethylenediammine cobalt(III)chloride and resolution of the cis form
Hexaminenickel(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
Bisethylenediaminenickel(II)chloride
Quantitative Analysis (Any 4 experiments)
Analysis involving volumetric and gravimetric estimations of mixtures of cations Cu & Ni; Cu & Zn; Zn & Cu; Fe & Ni; Fe(II) & Fe(III)

Text Books:

l. G., Svehla , 'Vogel's Qualitative Inorganic Analysis', 6th Edn., Orient Longman New Delhi, l987.
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.
4. Inorganic Synthesis, 34 Vols set
5. A. I. Vogel, Text Book of Quantitative Inorganic Analysis, 5th Edn, Longman, 1989

CH 612 – Physical Chemistry Practicals

1. Kinetic study of hydrolysis of ester. Determination of order, I^- and $S_2O_8^{2-}$.
2. Determination of partition co-efficient and equilibrium constant. $KI + I_2 \rightarrow KI_3$.
3. Kinetics of iodination of acetone by spectrophotometer.
4. Adsorption of oxalic acid on activated charcoal.
5. Determination of heat of solution and heat of fusion.
6. Study of three component system.
7. Partition coefficient of NH_3 between water and chloroform.
8. Determination of solubility product.
9. Partial molar volume of NaCl.
10. pH-metry
11. Conductometric titration of mixture of acids. Precipitation titration (KCl Vs $AgNO_3$) using conductivity bridge.
12. Potentiometric titrations

Semester 3

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.

Use of the following reagents in organic synthesis and 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.

Text Books:

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

References:

1. 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, M.O. 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.

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.

Text Books:

1. L.V. Azaroff " Introduction to solids" Mc.Graw hill, New York.
2. H. J. Arnikar, 'Essentials of Nuclear Chemistry', 4th Edn., New Age International Publishers Ltd., New Delhi, 1995.

References:

1. F. A. Cotton, Wilkinson, G. and Paul, L. Gaus, 'Basic Inorganic Chemistry', 3rdEdn., John Wiley & Sons, New York, l995.
2. J. D. Lee, 'Concise Inorganic Chemistry', 5th Edn., ELBS. with Chapman and Hall, London, 1996.
3. J. E. Huheey, Ellen, A. Keiter and Richard, 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 Plank's radiation Law.

Photochemistry: Absorption and emission of radiation, Franck Condon principle decay of economically 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 emission. Einstein transition probability- inversion of population –laser and masers. Flash photolysis: Chemi and thermoluminescence.

Surface Chemistry I: Surface Phenomena, Gibbs adsorption isotherm, solid-liquid interfaces, contact angle and wetting, solid-gas interface, physisorption and chemisorption, Freundlich, Langmuir, 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, Surface Area and Mechanism of Heterogeneous Catalysis, Phase Transfer Catalysis. Chemical Analysis of surfaces: Surface preparations-Spectroscopic Surface methods, electron spectroscopy, ion scattering spectrometry secondary ion scattering microscopy (SIMS)-Auger election spectroscopy- instrumentation and application. Electron stimulated micro analysis. Scanning probe microscopes.

Text Books:

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 Books, 1998.
3. S. Glasstone, Thermodynamics for chemists, Affiliated East West Press, 1965.

References:

1. B. C. McClelland, Statistical Thermodynamics, Chapman and Hall, 1973.
2. L. K. Nash, Elements of classical and statistical thermodynamics, Addison-Wesley, 1970.
3. K. K. Rohatgi - Mukkerjee, "Fundamentals of Photochemistry", Wiley Eastern Ltd., (1992).
4. P. K. Ghosh, 'Introduction to Photoelectron Spectroscopy', Wiley Interscience, 1983.

CH 619- Spectroscopy

Electromagnetic radiation and its interaction with matter-Born–Oppenheimer approximation-Rotational spectroscopy-Selection rules- Vibrational spectra of diatomic molecules- rotational character of vibrational spectra- Morse potential - selection rules- overtones-Fermi resonance-polyatomic molecules- modes of vibrations -Raman Spectroscopy-Fundamentals- Rotational Raman -Vibrational Raman spectra- Electronic spectroscopy: Atoms and Molecules- Different types of electronic transitions – Frank Condon Principle- Double bond equivalence-Applications of IR and UV-Visible spectroscopy

Nuclear Magnetic Resonance I- Concept and theory- Rotating frame and Laboratory frame-FT-Generation and detection of FID- Instrumentation- Relaxation phenomena, ^{1}H- NMR- chemical shift –Anisotropic effects- 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

Nuclear Magnetic Resonance II: ^{13}C-NMR –Chemical shifts and line intensities-Spin decoupling- NOE - 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-INADEQUATE–Interpretation of spectra- Introduction to Solid state NMR- cross polarization-WAHUHA

Electron Paramagnetic Resonance: Basic principles-hyperfine interaction- zero-field energy levels- CW ENDOR and TRIPLE-basic principles-Application to organic radicals and transition metal complexes- Pulse EPR basics- Model system for pulse EPR experiments- Pulse Schemes and Applications-nuclear modulation experiments- 2- pulse and 3- pulse ESEEM- HYSCORE-Davies and Mims ENDOR-TRIPLE- Interpretation of EPR parameters- Distance measurements using ELDOR. Imaging methods in Magnetic resonance-Principles and applications of Mossbauer spectroscopy-NQR spectroscopy

Mass spectroscopy: Methods of desorption and ionization (EI, CI, ESI, MALDI, FAB, TOF)-Instrumentation-Magnetic sector analysis-quadrupole instruments- 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 - Combined Problems and Case studies.

Text Books:

1. R. S. Macomber, A Complete Introduction to Modern NMR SPectroscopy, John Wiley & Sons ltd
2. Donald L. Pavia, Gary M. Lampman, George S. Kriz, James A. Vyvyan, Introduction to Spectroscopy, Brooks Cole

3. C. N. Banwell: Fundamentals of Molecular Spectroscopy, 4th edn. Tata McGraw Hill, 1996
4. J. M. Hollas, Modern Spectroscopy, 4th Edn, John Wiley & Sons, 1992.
5. R. S. Drago: Physical Methods for Chemists, Second Edition, Saunders College Publication

References:

1. J. A. Weil, J. R. Bolton, Electron Paramagnetic Resonance, Elementary Theory and Practical Applications, Wiely-Interscience,
2. A. Schweigher, G. Jeshcke, Principles of Pulse Electron Paramagnetic Resonance, Oxford University press
3. L. D. Field, S. Sternhell, J. R. Kalman, Organic Structures from Spectra, John Wiley & Sons, Ltd
4. M. Balci, Basic ^{1}H- and ^{13}C-NMR Spectroscopy, Elsevier
5. E. A. V. Ebsworth, D. W. H. Rankin, and S. Cradock, Structural Methods in Inorganic Chemistry, Blackwell Publications
6. D. N. Sathyanarayana, Introduction to Magnetic Resonance Spectroscopy, ESR, NMR, NQR, I. K. International, 2009

Semester 4

CH 616-Biochemistry (Elective)

Foundations of Biochemistry: Cellular foundations, Chemical, Physcial, Genetic and Evolutionary foundations, Amino Acid structure, Essential Amino Acids, aminoacid metabolism, proteins, primary structure, Hydrophobic Interaction , van der Waals Interactions and London Dispersion Forces, Secondary Structure, Protein Stability, Temperature-Sensitive Mutations, Ligand-Binding Specificity, Membranes and Membrane Protiens, General Structure, Function, the composition and transport across membranes, membrane dynamics, Movement of Ions and Molecules Across Membranes, Transport Across Membranes, The Nernst Equation

Enzyme mechanism**,** Active Site, Transition State, Catalysis, Lock and Key mechanism, Enzyme kinetics, Michaelis-Menten Equation, Inhibition, Allosterism and Cooperativity, The Monod-Wyman-Changeaux Model, Signal Transduction Pathways, Organization, Signals, Receptors, soluble Receptors, Transmembrane Receptors, Enzyme Coupled Receptors, G-Protein Coupled Receptors, Ion-Channel Coupled Receptors, Second Messengers

Nucleotides and nucleic acids, Expression of Genetic Information, DNA & RNA, Structure and stability. Information Metabolism, DNA Replication , Types of DNA Polymerase, Regulation of Information Metabolism , Transcription, Regulation of Transcription, High-Energy Phosphate Bonds and Translation , Recombinant DNA methodology, Restriction Analysis, Gels and Electrophoresis, Expression of genetic information, Cloning, Sequencing , Mutagenesis

Bioenergetics and metabolism, Glycolysis and gluconeogenesis and pentosephosphate pathway, Glycolysis Function, Gluconeogenesis Function, Glycogen synthesis and degradation, the citric acid cycle, Fatty acid catabolism, fatty acid synthesis and degradation, triglycerids and

phosopholipids synthesis, electron transport and oxidative phosphorylation, photophosphorylation, and ATP synthesis, Lipids, storage metabolism, aminoacid oxidation and production of urea, carbohydrate biosynthesis in plants and bacteria

Information and Integrating Metabolic Pathways, Genes and Chromosomes, ATP, Glucose, Storage Molecules, Metabolic States and Signals, Insulin, Glucagon, Epinephrine, Fat, Metabolic Movements of Fat, Tissue Cooperation, Liver, Muscle, Adipose, Brain, Connection of Storage Pools, Feeding, Fasting, Starvation, Interorgan Cycles, Cori Cycle, Alanine Cycle, Ketone Bodies, Urea Cycle, Purine metabolism, Pyrimidine metabolism, one carbon metabolism, oxidation states of carbon, glucose to pyruvate, TCA cycle.

Text Books:

1. H. F. Gilbert, Basic Concepts of Biochemistry, A Students Survival Guide, 2nd Edn, McGraw Hill, 1992.
2. L. Lehninger, Biochemistry, 4th Edn, 2000.

CH 618-Catalysis (Elective)

The Phenomenon Catalysis - Mode of Action of Catalysts - Classification of Catalysts - Comparison of Homogeneous and Heterogeneous Catalysis. Individual Steps in Heterogeneous Catalysis - Kinetics and Mechanisms of Heterogeneously Catalyzed Reactions (Langmuir–Hinshelwood, Eley–Rideal)- - Catalyst Concepts in Heterogeneous Catalysis- Catalyst Performance - Catalyst Deactivation and Regeneration - Characterization of Heterogeneous Catalysts.

Preparation and characterization methods: Catalyst preparation. Structured catalysts and zeolite. Synthesis of zeolites, - Isomorphic Substitution of Zeolites -Metal-Doped Zeolites - Applications of Zeolites and Mesoporous solids. Catalyst characterization by SEM, EDAX, XRD, XPS, Electron microscopy, Gas adsorption and other techniques.

Mehanisms of selected reactions - Acid catalysis and zeolites. Processing of petroleum and hydrocarbons. Catalytic oxidation. Synthesis gas and associated processes. Steam reforming. The water gas shift reaction. Methanation. Ammonia production. Nitric acid. Methanol and formaldehyde. Fischer-Tropsch. Catalysis for environmental protection and energy production. Three way catalysts for automobiles. hydrogenation and dehydrogenation reactions - dehydration of alcohols - olefin hydrogenation - decomposition of nitrous oxide - oxidation of CO- ketonization of carboxylic acids, cracking of hydrocarbons.

Green Chemistry and Catalysis- Catalysts for PTC - Mechanism and Benefits of PTC -PTC Reactions - Selected Industrial Processes with PTC. Automotive Exhaust Catalysis - NOx and SOx Removal Systems -. Examples of catalytical process, Photocatalysis Basic Principles - Photoreduction and Oxidation of Water - Photocleavage of Water. Introduction to Biocatalysis - Kinetics of Enzyme-catalyzed Reactions -Industrial Processes with Biocatalysts. Introduction to Electrocatalysis and fuel cells.

Industrial application of catalysis- Petroleum Refining – Distillation, Cracking, Reforming, Hydrotreating, Alkylation and Isomerization, Steam Cracking. Ethylene-Based Processes - Ethylene Oxide and Ethylene Glycol, Polyethylene, Vinyl Chloride and PVC. Propylene-Based Processes - Acrylic Acid and Acrylonitrile, PP and Ziegler-Natta Chemistry. C4-Based Processes – Butadiene, Isobutylene, BTX Processes - Styrene and Polystyrene, Polyethylene Terephthalate (PET), Phenol, Adipic Acid and Nylon, Phthalic Anhydride

Text Books:

1. Emmett, P.H. - " Catalysis Vol.I and II, Reinhold Corp. ", New York, 1954.
2. Smith, J.M. - " Chemical Engineering Kinetics ", McGraw Hill, 1971.

References:

1. Thomas and Thomas " Introduction to Hetrogeneous Catalysts ", Academic Press, London 1967.
2. Jens Hagen – "Industrial Catalysis: A Practical Approach", 2nd Edition, WILEY-VCH, March 2006.
3. H. Bartholomew, Robert J. Farrauto, "Fundamentals of Industrial Catalytic Processes", 2nd Edn; Wiley. 2006

CH 620- Computational Chemistry (Elective)

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, Goto 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.

Text Books:

1. K. V. Raman, 'Computers in Chemistry', Tata McGraw Hill, 1993.
2. F. Jensen, 'Introduction to Computational Chemistry', John Wiley & Sons, 2003.

References:

1. C. Balagurusamy, 'Programing in C', Tata McGraw Hill, 1997.
2. M. K. Jain, 'Numerical Methods for Scientific and Engineering Computation', Wiley Eastern Ltd, 1995.
3. User manuals of Gaussian03, Chemoffice Ultra and Gauss View

CH 622-Electron Spectroscopy (Elective)

Photoelectric effect: basic principles of electron spectroscopy, classification of various spectroscopies.

Photoelectron spectroscopy: experimental methods-electron energy analysis-photon sources -- UV, X-ray, synchrotron, theory, angular dependence-cross section and its determination-valence and core photoemission - Koopmans' theorem- supersonic molecular beam spectroscopy - coincidence studies, photoelectron diffraction, band structure, holography, circular dichroism.

Electron energy loss spectroscopy: Franck and Hertz experiment -- instrumentation -selection rules-theory - studies on molecules - surface states - high resolution spectroscopy - adsorption and catalysis -applications.

Auger electron spectroscopy: introduction - instrumentation - classification of various transitions - quantitation - applications - Auger microscopy.

Related techniques: inverse photoemission - multiphoton ionization - electron momentum spectroscopy - photoionization- photo detachment - zero kinetic energy photoelectron spectroscopy - spin resolved photoemission - recent advances in instrumentation-brighter photon sources.

References:

1. P. K. Ghosh, 'Introduction to Photoelectron Spectroscopy', Wiley Interscience, 1983.
2. K. Seigbahn et.al., ESCA applied to Free Molecules", North Holland Publishing Company", 1969.
3. A. D. Baker and C. R. Brundle, Eds, "Electron Spectroscopy" Vol. 1 - 4 Academic Press, 1978.
4. J. W. Rabalais, "Principles of Ultraviolet Photoelectron Spectroscopy". Wiley- Interscience, 1975
5. J. Berkowiz, "Principles of Ultraviolet Photoelectron Spectroscopy". Academic Press, 1975

CH 624 - Environmental Chemistry (Elective)

Scope- Environmental Pollution- Structure of atmosphere- Biogeological cycles - Oxygen-Nitrogen-Carbon-Phosporous- Sulfur- 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 - Cimatic 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-Ca-Mg-Fe-Mn-Hg-Ag-An-Cr-As-Ammonia-Nitrite-Nitrate-Fluoride-Sulfide-Phosphate-Be-Cd-Cu-Pb-Se-Phenols-Surfactants-BOD-COD-DO-TOC-Nondispersive IR spectroscopy-Anode stripping-ICPAES-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

Text Books:

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
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 626 - Medicinal Chemistry

Introduction to the 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 of 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 and mechanism, kinetic, spectroscopic, isotopic and stereochemical studies. Chemical models and mimics for enzymes, Design, synthesis and evaluation of enzyme inhibitors

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

Text Books:

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.

References:

1. Bentley and Driver's Text Book of Pharmaceutical Chemistry revised by L.M. Artherden, Oxford University Press, London, 1977.
2. A. Gringauz, Introduction to Medicinal Chemistry, How drugs act and why, John Wiley and sons, 1997
3.G. L. Patrick, Introduction to Medicinal Chemistry, Oxford Univeristy Press, 2001

CH 628- Nano Science and Technology (Elective)

Introduction to Nanoscience: Introduction - definition of nanoscience, nanochemistry - classification of the nanomaterials – zero dimensional nano structures - one dimensional nanostructures – nanowires and nanorods – two dimensional nanostructures – films, nanotubes

and biopolymers – three dimensional nanostructures – fullerenes and dendrimers - quantum dots and their properties. Basic instrumentation and imaging techniques.

Synthesis of Nanomaterials: Introduction - precipitative methods - reactive methods in high boiling point solvent - hydrothermal and solvothermal methods - gas phase synthesis of semiconductor nano- particles – water based gold nanoparticle synthesis - organic solution based synthesis-sonochemical methods and microwave methods. CNTs and CNFs

Properties of nanomaterials : Electronic Structure of Nanoparticles. Electronic properties and thermal properties. Melting point and phase transition processes- quantum-size-effect (QSE). Size-induced metal-insulator-transition (SIMIT)- nano-scale magnets, transparent magnetic materials, and ultrahigh-density magnetic recording materials-chemical physics of atomic and molecular clusters.

Chemistry Aspects Photochemistry; Photoconductivity; Electrochemistry of Nanomaterials-Diffusion in Nanomaterials; Nanoscale Heat Transfer; Transport in Semiconductor Nanostructures; Transition Metal Atoms on Nanocarbon Surfaces; Nanodeposition of Soft Materials; Nanocatalysis, Catalysis by gold and silver Nanoparticles;

Nanostructures- Kinetics in Nanostructured Materials- Zero dimensional, one-dimensional and two dimensional nanostructures- clusters of metals and semiconductors, nanowires, nanostructured beams, and nanocomposites-artificial atomic clusters-Size dependent properties-size dependent absorption spectra-phonons in nanostructures.

Text Books

1. T. Pradeep, Nano: The Essentials, Tata McGraw-Hill, New Delhi, 2007.

References

1. G. Cao, Nanostructures and Nanomaterials – Synthesis, Properties and Applications, Imperial College Press, London, 2004, chapters 3, 4 and 5.
2. C. N. R.Rao, A. Muller and A. K. Cheetham, The Chemistry of Nanomaterials, Volume 1, Wiley –VCH Verlag GmbH & Co. KgaA, Weinheim, 2004,c Chapter 4.

CH 630- Natural Products Chemistry

Aminoacids: Synthesis of amino acids-reactions - properties- Amino Acids in Nature: β-Amino Acids and their Metabolites in Nature – Taxonomy of the Producer Organisms- Seebach's Nomenclature- Properties-Synthesis and biosynthesis of β-aminoacids. Structure of proteins-Peptides, *In vitro* and *in vivo* synthesis of peptides-bradykinin, oxytocin, vasopressins, gramicidins. Juvenile hormone cecropia juvenile hormone, Insect pheramons

Steroids– classification- Synthesis and structure elucidation of cholesterol, conversion of cholesterol to progesterone- androsterone and testosterone-cortisone- Vitamin D - Purins and Nucleic Acids- nucleosides and nucleotides-RNA and DNA, Watsons and Creig model. Elucidation of enzyme structure and mechanism - chymotrypsin, NAD- DNA-protein interaction and DNA-drug interaction

Lipids: Prostaglandins, Vitamins - thromboxane Tx- Pyridoxol, - carotenes- Vitamin A- Vitamin B complex- biotin-Vitamin E and K group- Xanthophylls-Biosynthesis of carotenes- Penicillins, Cephalosporin- C, -Tetracyclins- affotoxins B1 and M1, pseudonomic acid A and B.

Classification of natural products: chemical structure, physiological activity, taxonomy and biogenesis-Alkaloids – classification, structure elucidation based on degradative reactions-synthesis of quinine, morphine, papaverine, and reserpine- Anthocyanins, flavones and isoflavones, examples in each family. Plant Harmones, gibberllins, gibberellic acid

Terpenoids: classification, Citral, juvabione, transchrysanthamic acid, logifolene, taxines, caryophyilene structure elucidation and synthesis of abietic acid- Carbohydrates: Determination of configuration- Hudsons rules-Structure of sugars- transformation of sugers, Preparation of alditols, glycosides, deoxysugars. Synthesis of vitamin C from glucose.

Text books:

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.

References

1. Atta-ur-Rahman, Studies in Natural Products Chemistry, Vol.1 and 2, Elsevier, 1988.
2. R. Krishnaswamy: Chemistry of Natural Products; A Unified Approach, Universities Press
3. R. J. Simmonds: Chemistry of Biomolecules: An Introduction, RSC

CH 632 Novel Inorganic Compounds (Elective)

Acyclic & cyclic systems from the periodic table - Inorganic homo- & heterocycles saturated and unsaturated ring systems, p-electron precise and rich rings. synthesis, structure and reactivity.

Metallocycles - Chemistry of individual rings.

Cages & clusters of elements, structural variety, properties and implications of borides, carbides, silicides, nitrides, phosphides, oxides and sulphides of transition elements, multiple bonds and cluster variety of transition metals.

Higher boranes, carboranes and metalloboranes.

Inorganic 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. F. A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, John Wiley, 1988.
4. I. Haiduc & D. B. Sowerby (Eds.), Inorganic Homo-and Heterocycles Vols. 1 & 2, Academic Press, 1987.
5. J. E. Mark, R. West & H. R. Allcock, Inorganic Polymers, Acad.Press, 1992.

CH 634 - Nuclear Chemistry (Elective)

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.

Bethe notation-Types of nuclear reactions: 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.

Text Books:

1. Walter Loveland, David Morrissey, Glenn 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.

References:

1. K. H. Lieser, Nuclear and Radiochemistry, 2nd revised ed., Wiley-VCH, Berlin, 2001.
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Concept of macromolecules-Principle of duality- Molecular design-Tetrahedral model of product development. Nomenclature and Classification- Raw Material sources of polymers- Synthetic schemes- Petroleum and petrochemicals- Oil Refinery: a perceptive-. Naphtha as a source of petrochemicals.

Polymerization processes. Free radical addition polymerization. Kinetics and mechanism. Chain transfer- Molecular weight distribution and molecular weight control. Radical Atom Transfer and Fragmentation – Addition mechanism. Free radical living polymers. Cationic and anionic polymerization. Kinetics and mechanism, Polymerization without termination. Living polymers. Step Growth polymerization- Linear Vs cyclic polymerization, other modes of polymerization- Copolymerization- 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 and dynamic methods, Light scattering and GPC. Crystalline and amorphous states. Glassy and Rubbery States. Glass transition and crystalline melting. Spherullites and Lammellac. Degree of Crystallinity, X-ray diffraction, Thermal analysis of polymers. TG/DTG, DTA/DSC, DMA/TMA/DMTA

Polymer Solutions - Flory-Huggins equation - Chain dimension-chain stiffness – End-to-end distance- Conformation-random coil- Solvation and Swelling- Flory-Reiner equation. 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. Polymers with high bandwidth. Polyanilines, polypyrrols, polythiophines, poly(vinylene phenylene). Photoresponsive and photorefractive polymers. Polymers in optical lithography. Polymer photoresists. Electrical and NLO properties of Polymers, Polymers - wave guide devises.

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