National Institute of Technology, Jamshedpur

Department of Chemistry

M.Sc. Chemistry

Credit Structure

Course Work	Sem I	Sem II	Sem III	Sem IV
Core Course	22	22	22	-
Electives	-	-	-	12
Project /Dissertation	-	-	-	12
Credit	22	22	22	24
Total Credit		90		

COURSE STRUCTURE
Department of Chemistry
M. Sc. Chemistry

Ist Year

FIRST SEMESTER

Sl. No.	Course Code	Course Title	L-T-P	Credits
1	CHG5111	Thermodynamics and Electrochemistry	3-1-0	4
2	CHG5112	Physical Organic Chemistry	3-1-0	4
3	CHG5113	Transition and Inner-Transition Elements	3-1-0	4
4	CHG5114	Analytical Chemistry	3-1-0	4
5	CHG5115	Physical Chemistry Laboratory	0-0-12	6
		Total Credits		22

SECOND SEMESTER

Sl. No.	Course Code	Course Title	L-T-P	Credits
1	CHG5116	Quantum Chemistry	3-1-0	4
2	CHG5117	Photochemistry and Pericyclic Reactions	3-1-0	4
3	CHG5118	Organometallic Chemistry	3-1-0	4
4	CHG5119	Instrumentation Techniques in Chemistry	3-1-0	4
5	CHG5120	Inorganic Chemistry Laboratory	0-0-12	6
		Total Credits		22

2nd Year

THIRD SEMESTER

Sl. No.	Course Code	Course Title	L-T-P	Credits
1	CHG6121	Chemical Kinetics and Molecular Spectroscopy	3-1-0	4
2	CHG6122	Reaction Mechanism and Retrosynthesis	3-1-0	4
3	CHG6123	Applied Chemical Analysis	3-1-0	4
4	CHG6124	Solid State Chemistry	3-1-0	4
5	CHG6125	Organic Chemistry Laboratory	0-0-12	6
		Total Credits		22

FOURTH SEMESTER

Sl. No.	Course Code	Course Title	L-T-P	Credits
1		Elective	3-1-0	4
2		Elective	3-1-0	4
		Elective	3-1-0	4
3	CHG6151	Project	0-0-12	12
		Total Credits		24

SUMMARY

Semester	I	II	III	IV
Credit per semester	22	22	22	24
Total Credits	90			

List of Electives

Sl. No.	Course Code	Subject Name
1.	CHG6126	Environmental Chemistry
2.	CHG6127	Supramolecular Chemistry
3.	CHG6128	Industrial Chemistry
4.	CHG6129	Nanochemistry
5.	CHG6130	Corrosion Science and Engineering
6.	CHG6131	Computational Chemistry
7.	CHG6132	Polymer Chemistry
8.	CHG6133	Nuclear Chemistry
9.	CHG6134	Natural Products
10.	CHG6135	Methods in Organic Synthesis
11.	CHG6136	Surface Chemistry
12.	CHG6137	Photochemistry and Its Applications
13.	CHG6138	Advanced Quantum Mechanics
14.	CHG6139	Advanced Magnetic Materials

1st Semester

CHG5111: Thermodynamics and Electrochemistry (4 credits: 3-1-0)

Classical Thermodynamics: Laws of thermodynamics. Thermodynamic functions and their relationships: Gibbs-Helmholtz and Maxwell relations, Van't Hoff equation. Criteria of spontaneity and equilibrium. Evaluation of absolute entropies. Partial Molar Properties, Chemical potential and its variation with temperature and pressure, Fugacity.

Statistical Thermodynamics: Introduction: Concept of ensembles, partition functions and distributions, microcanonical, canonical and grand canonical ensembles, canonical and grand canonical partition functions, Boltzmann, Fermi-Dirac and Bose-Einstein distributions. Gibbs paradox and Sackur – Tetrode equation. Concept of thermal wavelength. Molecular partition functions – transitional, rotational, vibrational, electronic, nuclear. Equipartition theorem and its validity. Chemical potential and chemical equilibrium – Saha ionisation formula. System of interacting molecules – Imperfect gas. Specific heat of electron gas, Bose condensation. Liouville theorem and its consequences, its quantum version. Formulation of Quantum statistics – density matrix.

Electrochemistry: 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. Electrical Double layer: Theories of Double-Layer structure, diffuse-double-layer theory of Gouy and Chapman, the Stern Model. Polarization and Overvoltage. Current-potential relationship (derivation of Butler-Volmer and Tafel equations). Electrochemical energy systems: Secondary cells, Fuel cells.

Text Books/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. J. O. M. Bockris and A. K. N. Reddy, Modern Electrochemistry, Plenum Press, 1970.
4. J. Rajaram & J. C. Kuriacose, Thermodynamics for Students of Chemistry, Shobanlal Nagin Chand Co, 1986
5. K. L. Kapoor, A Text Book of Physical Chemistry, Volumes 2 and 5, 3rd Edition, Macmillan India Ltd, 2004.

CHG5112: Physical Organic Chemistry (4 credits: 3-1-0)

Stereochemistry: Introduction to molecular symmetry and chirality, The concept of stereochemistry and absolute and relative configurations, Different nomenclatures, interconversion of Fischer, Newman and Sawhorse projections The concept of prochirality: topicity, prosteroisomerism, stereotopic ligands and faces and stereoheterotopic ligands, Center of chirality, molecules with C, N, S based chiral centers, axial, planar and helical chirality, stereochemistry and absolute configuration of allenes, biphenyls, binaphthyls, spiranes, exo-cyclic alkylidenecycloalkanes, ansa and cyclophanic compounds. Racemic modifications. Desymmetrization and kinetic resolution, methods of determination of absolute configuration.

Conformational Analysis: Introduction to conformational analysis, steric, conformation around sp^3-sp^2 and sp^2-sp^2 bond, electronic and stereoelectronic effects in governing the conformation of acyclic and cyclic (5 and 6 membered rings) systems, A-strains and anomeric effect, decalins, transannular interactions in medium size rings.

Conformation and Reactivity: steric and electronic effects in syn-elimination, E2 elimination and neighboring group participation (Woodward, Prevost methods) of acyclic and cyclohexyl systems, esterification, substitution reaction and formation and opening of epoxide in cyclohexyl systems (Furst Plattner rule).

Physical Organic Chemistry: Optical rotatory dispersion (ORD) and circular dichroism (CD), classification of ORD and CD Curves, Cotton effect curves and their application to stereochemical problems; the Octant rule and its application to alicyclic ketones. Relationship between thermodynamic stability and rates of reactions – kinetic and thermodynamic control of product formation, Hammond's postulate, Curtin Hammett principle, steric effects: Taft equation,. Catalysis (acids, bases, and nucleophiles) and isotope effects, importance in the determination of organic reaction mechanisms, solvent effects, examples from SN2 and E2 reactions. Introduction to carbon acids, pKa of weak acids.

Text Books/Reference:

1. Organic Chemistry by Clayden, Greeves, Warren and Wothers: Oxford University Press.
2. Advanced Organic Chemistry by J. March and M. B. Smith: Wiely-Interscience
3. Stereochemistry of Organic Compounds by D. Nasipuri.

4. Advanced Organic Chemistry: Structure and Mechanism by F. A. Carey and R. J. Sundberg: Plenum Publishers.

CHG5113: Transition and Inner-Transition Elements (4 credits: 3-1-0)

Theories of Bonding: VBT and its limitations, CFT; Spitting of *d* orbitals in crystal fields of different symmetry for similar and dissimilar ligands (Octahedral, tetrahedral, Linear, trigonal planar, trigonal bipyramidal, square pyramid), crystal field stabilization energies (CFSE) and pairing energy, spectrochemical series, JT-distortion, Low spin and high-spin complexes. Thermodynamic aspects of crystal field splitting (variation of ionic radii, lattice energy, hydration enthalpy and stability constants of complexes –Irving Williams order). Kinetic aspects of crystal field stabilization: crystal field activation energy, labile and inert complexes. Nephelauxetic series. Limitation of CFT. LFT. Molecular Orbital Theory, MO of diatomic and polyatomic molecules (N_2, CO, BeH_2, H_2O, B_2H_6, octahedral, tetrahedral and square planar complexes).

Electronic Spectra: d-d transitions, Orgel and Tanabe-Sugano diagrams, charge-transfer spectra. Magnetism; Types, determination of magnetic susceptibility, spin-only formula, spin-orbit coupling, spin crossover.

Lanthanides and Actinides: Contraction, coordination, optical spectra and magnetic properties**,** redox chemistry, analytical applications.

Text Books/Reference:

1. James E. Huheey, Inorganic Chemistry - Principles of Structure and Reactivity, 4th Edition, Pearson Education, 2006.
2. Stephen J. Lippard and Jeremy M. Berg, Principles of Bioinorganic Chemistry, 2nd Edition, Panima Publishing Corporation, 2005.
3. Cotton and Wilkinson Advanced Inorganic Chemistry, Wiley Eastern, 1976.
4. D. F. Shriver, P. W. Atkins and C. H. Langford, Inorganic Chemistry, Oxford University Press, 1990.
5. Inorganic Chemistry by J. D. Lee.

CHG5114: Analytical Chemistry (4 credits: 3-1-0)

Errors and Statistical Treatment of Data: Accuracy and precision, errors, Statistical treatment of data, error distributions, finite data analysis, standard deviation, criteria for rejection of data, method of least squares. Infrared Spectroscopy: Basic concepts, Characteristic vibrational frequencies of organic compounds and factors affecting stretching frequencies. UV Spectroscopy: UV-Visible, Basic concepts and factors affecting the position of UV bands, Characteristic absorption of Organic compounds, Application of UV spectroscopy. Mass Spectroscopy: Mass spectral fragmentation of organic compounds, McLafferty rearrangements, Applications. Nuclear Magnetic Resonance Spectroscopy: Basic Concepts, chemical shifts, spin-spin interaction, Fourier transform technique and nuclear Overhauser effect (NOE). Coupling constants, two-dimensional NMR spectroscopy, NOESY, DEPT and INEPT terminologies. Structural elucidation of organic compounds using UV, NMR, IR and Mass spectroscopy. 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. Thermogravimetry, Differential Thermal Analysis (DTA), and Differential Scanning Calorimetry (DSC).

Text Books/Reference:

1. Analytical Chemistry: (J.W) G. D. Christain
2. Introduction to Spectroscopy, 5th Edition, by Donald l. Pavia, Gary M. Lampman, George A. Kriz, and James R. Vyvyan
3. Modern Analytical Chemistry, David Harvey, McGraw Hill, 2000.
4. Organic Spectroscopy, Kemp W.
5. Treatise on Analytical Chemistry: Vol Ito VII – I. M. Kolthoff
6. Spectroscopic identification of organic compounds- R.M. Silverstein and G. C. Bassler
7. Spectroscopic methods in organic chemistry- D.H. Williams and I. Fleming
8. Absorption spectroscopy of organic molecules- V.M. Parikh
9. Applications of spectroscopic techniques in Organic chemistry- P. S. Kalsi
10. A Text book of Qualitative Inorganic Analysis- A. I. Vogel

CHG5115: Physical Chemistry Laboratory (6 credits: 0-0-12)

Conductometric titrations: Dissociation constant of weak acid, solubility product of sparingly soluable salt ($PbSO_4$, $BaSO_4$), Determination of strength of strong and weak acids in a given mixture conductrometrically, Determination of ratio of Potassium Dichromate, chromate in a supplied mixture. Potentiometric titration: Determination of Dissociation Constant of weak acid Determination of pH of an electrolyte. Polarimetric determination of Concentration of unknown sugar solution Inversion of cane sugar; Determination of Co-ordination number of copper in cupramine complex by distribution method, determination of Equilibrium constant of the reversible reaction KI + I2 = KI3, Kinetics of Easter Hydrolysis by acid and base; Determination of Molecular mass of volatile liquids by Victor Meyer Method. Determination of Molecular mass of inorganic solids by Rast's method, Determination of magnetic moment by Gouy's balance.

Text Books/References:

1. B. Behera, Experimental Physical Chemistry, Tata McGraw Hill 2000.
2. D. Alart, Practical Physical Chemistry, Longman, 1993.

2nd Semester

CHG5116: Quantum Mechanics and Its Application (4 credits: 3-1-0)

Inception of quantum mechanics (Black body radiation, Planck's quantum theory), Photoelectric effect, Compton effect (Introductory part). Double slit experiment, Phase Velocity and Group velocity ,Wave packets, Wave–Particle duality (de-Briglie's hypothesis). Non-relativistic and relativistic particles and its relation with wavelength and momentum. Heisenberg's Uncertainty Principle (Derivation), Postulates of quantum mechanics, Mathematical tools of quantum mechanics (Linear and Hilbert vector space), Dirac Notations, Operators (definition, properties, examples), Commutation relations, Hermitian Operator and its properties, Unitary operator, Projection operator, Parity operator, Virial Theorem. Eigen functions and eigenvalues of operators and superposition principle. and expectation values. Schrodinger equation (time independent and time dependent with derivation); Probability concept, Time evolution of probability, Ehrenfest's theorem, Superposition of wave functions, Expectation value of observable. Current density probability. Particle in a 1D, 2D and 3D box (Derivation), degeneracy, Particle in a finite box, Step potential, rectangular box, Tunneling effect, utility of particle in a box model.

Harmonic oscillator, Angular momentum, Eigen values of angular momentum operator, ladder operators, orbital and spin motion of electron, coupling of angular momenta including spin-orbit coupling, valence bond and molecular orbital methods, polyatomic molecules. Huckle Theory, Hydrogen Atom solution using Schrodinger equation. Time-independent perturbation theory, degenerate states, variational method, Hellmann-Feynman theorem Spectra and structure of helium atom, term symbols for atoms and molecules.

Text Books/References:

1. Nouredine Zettili, Quantum Mechanics (Concept and Applications) 2nd Edition.
2. G. Arfken and Hans J. Weber, Mathematical methods for physicists.
3. D. A. McQuarrie, Quantum Chemistry, University Science Books, 1983.
4. P. W. Atkins, Molecular Quantum Mechanics, 2nd edition.
5. I. N. Levine, Quantum Chemistry, 3rd edition.
6. D. J. Griffiths, Introduction to Quantum Mechanics, 2nd Edition.
7. Rbert Eisberg and Robert Resnik. Quantum Physics of Atoms, Mlecules Solids, Nuclei and Particles, 2nd Edition.
8. John Powel and Bernd Crasemann, Quantum Mechanics

CHG5117: Photochemistry and Pericyclic Reactions (4 credits: 3-1-0)

Concerted Reactions: Conservation of orbital symmetry, Woodward and Hoffmann rules. Orbital correlation, FMO and PMO treatments to electrocyclisation, cycloaddition, sigmatropic rearrangements and other related concerted reactions such as cyclo-additions and cyclo-reversion reactions, electrocyclic reaction and the electroreversion reactions, sigmatropic reactions, group transfer reaction.

Photochemical Reactions Basic principles of Photochemical reactions, Photochemistry of alkenes, carbonyl compounds, and arenes. Norrish type I process, Norrish type II process. Photooxidation and photoreduction. Di-π- methane rearrangement, Barton reaction, Paterno Buchi reaction, Nazarov cyclization. Cis-trans isomerisation, Chemistry of vision

Free Radical Reaction

Types of free radical reactions, free radical substitution mechanism, mechanism at an aromatic substrate, neighboring group assistance, Reactivity for aliphatic and aromatic substrates, Reactivity in the attacking radicals, the effect of solvents on reactivity, Allylic halogenation, Oxidation of aldehydes to carboxylic acids, auto-oxidation, Sandmeyer reaction, free radical rearrangement, Hunsdiecker reaction.

Text Books/ Reference:

1. Heterocyclic Chemistry by T. L. Gilchrist, Pearson Education, 3rd Ed. 2007.

2.Photochemistry & Pericyclic Reactions by J. Singh & J. Singh, New Age International (P) Ltd., 2007.

3. Frontier Orbitals and Organic Chemical Reactions by I. Fleming, Wiley, 1976.

4. Organic Chemistry by Clayden, Greeves, Warren and Wothers: Oxford University Press.

CHG5118: Organometallics and Bio-inorganic chemistry (4 credits: 3-1-0)

Structure and Bonding: Structure and Bonding: Introduction, 18 electron rule, application to π- acceptor ligands, limitations. 16 electron rule, examples. Synthesis and reactivity of metal carbonyls, vibrational spectra of metal carbonyls. Metal- metal bonds and metal atom clusters. Types of M-C bonds; synthesis and reactivity of metal alkyls, carbenes, alkenes, alkynes, and arene complexes. Metallocenes and bent metallocenes. Structure and bonding in Zeise's salt, bis-(triphenylphosphine) diphenylacetylene platinum (0), diallyl nickel, ferrocene and dibenzene chromium(0). Isolobal analogy. Bonding and important reactions of metal nitryl, dinitrogen and dioxygen complexes, tertiary phosphine and NHC

complexes.

Structure and Bonding: Introduction, 18 electron rule, application to π- acceptor ligands, limitations. 16 electron rule, examples. Synthesis and reactivity of metal carbonyls, vibrational spectra of metal carbonyls. Metal- metal bonds and metal atom clusters. Types of M-C bonds; synthesis and reactivity of metal alkyls, carbenes, alkenes, alkynes, and arene complexes. Metallocenes and bent metallocenes. Structure and bonding in Zeise's salt, bis-(triphenylphosphine) diphenylacetylene platinum (0), diallyl nickel, ferrocene and dibenzene chromium(0). Isolobal analogy. Bonding and important reactions of metal nitryl, dinitrogen and dioxygen complexes, tertiary phosphine and NHC complexes.

Reactions of Organometallics: Substitution, oxidative addition, reductive elimination, insertion and deinsertion. Catalysis - Hydrogenation, Hydroformylation, Monsanto process, Wacker process, Alkene polymerization (Zeigler-Natta Catalyst), Reppe catalyst.

Boranes and phosphazenes.

Bio-inorganic Chemistry: Oxygen transport; Hemoglobin, myoglobin, hemerythrin, hemocyanin. Vitamin B_{12} and coenzymes. Electron- transfer reactions; nitrogen fixation, metal complexes in medicine. Photosystems and porphyrins.

Text Books/References:

1. James E. Huheey, Inorganic Chemistry - Principles of Structure and Reactivity, 4th Edition, Pearson Education, 2006.

2. Stephen J. Lippard and Jeremy M. Berg, Principles of Bioinorganic Chemistry, 2nd Edition, Panima Publishing Corporation, 2005.

CHG5119: Instrumentation Techniques in Chemistry (4 credits: 3-1-0)

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. CHN analysis by GC- other elemental analysis methods. 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.

Text Books/References:

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
3. F. Rouessac and A. Rouessac, Chemical Analysis: Modern Instrumentation
4. Methods and Techniques, 2nd edn, John Wiely and Sons
5. D. A. Skoog, E. J. Holler, S. R. Crouch , Principles of Instrumental Analysis, 6th edition,
6. Thomson Brooks Cole , 2007
7. F. W. Fifield and D. Kealey, Principles and Practice of Analytical Chemistry, 2nd Edition,
8. International Book Company, London, 1983
9. H. H. Willard, L.L. Merrit, J.A. Dean and F.A. Settle, Instrumental Methods of Analysis, D, CBS Publishers, New Delhi, 1986
10. Introduction to chromatography : Bobbit
11. Instrumental Methods of Analysis : Chatwal and Anand
12. Instrumental Methods of Inorganic Analysis(ELBS) : A.I. Vogel
13. Chemical Instrumentation: A Systematic approch- H.A. Strobel
14. The principals of ion-selective electrodes and membrane transport: W.E.Morf

CHG5120: Inorganic Chemistry Laboratory (6 credits: 0-0-12)

Qualitative analysis and quantitative estimations of radicals (PO_4^-, NO_3^-, SO_4^-, NH_4^+, Ca^{2+}, Mg^{2+} etc.) (Polarography, Amperometry & Biamperometry, Potentiometry, spectrophotometry, Turbidimetry, Electrogravimetry, pH metry and Flame photometry), synthesis (air-sensitive, moisture-sensitive etc.,), characterization and property measurements of inorganic (especially coordination) compounds, Exposure to various spectroscopic characterization techniques.

Text Books/References:

1. G. Svehla, Vogel’s qualitative inorganic analysis, Harlow Longman, 2002.

2. A. I. Vogel, John Bassett, Vogel's textbook of quantitative inorganic analysis: including elementary instrumental analysis, Longman, 2003
3. A. I. Vogel, Qualitative Inorganic Analysis, Orient Longman – 1979.

3rd Semester

CHG6121: Molecular Spectroscopy and Chemical Kinetics (4 credits: 3-1-0)

Molecular Spectroscopy and Group Theory

Interaction of radiation with matter, Einstein coefficients, time dependent perturbation theory, transition probability, transition dipole moments and selection rules, factors that control spectral linewidth and lineshape. Beer-Lambert law and absorbance.

The rigid diatomic rotor, energy eigenvalues and eigenstates, selection rules, intensity of rotational transitions, the role of rotational level degeneracy, the role of nuclear spin in determining allowed rotational energy levels. Classification of polyatomic rotors and the non-rigid rotor. Vibrational spectroscopy, harmonic and anharmonic oscillators, Morse potential, mechanical and electrical anharmonicity, selection rules. The determination of anharmoncity constant and equilibrium vibrational frequency from fundamental and overtones. Normal modes of vibration, G and F matrices, internal and symmetry coordinates. Electronic transitions, Franck-Condon principle. Vertical transitions. Selection rules, parity, symmetry and spin selection rules, Fermi Golden Rule. Polarization of transitions. Fluorescence and phosphorescence. Raman spectroscopy, polarizability and selection rules for rotation and vibrational Raman spectra. Non-linear scattering hyper Raman, stimulated Raman, Resonance Raman Spectra. Symmetry elements and operations, point groups, group multiplication table, matrix representation of symmetry operations. Representations using different basis, reducible and irreducible representations, construction of irreducible representation, great orthoganality theorem (GOT). Construction of character tables (C_2v, C_3v, C_2h and C_4v), Mülliken symbols, reduction formula, direct sum and direct products, connection between group theory and quantum mech

Chemical Kinetics

Theories of Reaction Rates: Potential energy surfaces-adiabatic and non-adiabatic curve crossing Processes- transition state theory- activation/thermodynamic parameters. Various theories of Unimolecular reactions (Lindemann- Christiansen hypothesis; Hinshelwood, RRK and RRKM theories; non RRKM behavior)

Kinetics in the Excited State: Jablonski diagram. Kinetics of Unimolecular and bimolecular photophysical and photochemical processes. Resonance energy transfer rates-Fluorescence quenching kinetics in solution and gas phase.

Activation and diffusion controlled processes- Marcus kinetics and quadratic dependence of Gibbs free energies-electron transfer processes involving organic and inorganic compounds.

Text Books/References:

1. C. N. Banwell and E. M. McCash, Fundamentals of Molecular Spectroscopy, 4th Edition.
2. J. Michael Hollas, Modern Spectroscopy, 4th Edition
3. Chemical Kinetics and Dynamics; Jeffrey I Steinfeld, Joseph S. Francisco and William L. Hase. Prentice Hall, 2nd edition, 1998.
4. Laidler, K. J.; "Chemical Kinetics", 3rd Edition 1997 , Benjamin-Cummings. Indian reprint - Pearson 2009.
5. Laser Spectroscopy- Basic concepts and instrumentation – W. Demtroder (Springer 3rd edition, 2004).
6. K. K. Rohatgi - Mukkerjee, "Fundamentals of Photochemistry", Wiley Eastern Ltd., 1992.
7. F. A. Cotton, Chemical Applications of Group Theory, Wiley, 1996.
8. Daniel C Harris and Michael D. Bertlucci, Symmetry and Spectrscopy.

CHG6122: Reaction Mechanism and Retrosynthesis (4 credits: 3-1-0)

Reagent type and reaction type, Investigation of reaction mechanism (nature of products, kinetic data, use of isotope, study of intermediate, stereochemical criteria.Types of mechanisms, types

of reactions, thermodynamic and kinetic requirements, free energy relationships, kinetic and thermodynamic control, Nature of reaction energy, Potential energy diagrams, transition states

Stereoselectivity: Classification, terminology, principle of stereoselectivity, examples of diastereoselectivity using Cram, Cram-Chelate, Felkin-Ahn, anti-Felkin, Houk models, Cieplak and cation coordination models, and Zimmerman-Traxler transition states, enantioselectivity.

C-X bond (X = C, O, N) formations through the intermediacy of Carbanions: Chemistry of enolates and enamines, Kinetic and Thermodynamic enolates, Lithium and boron enolates in

aldol and Michael reactions, Alkylation and acylation of enolates, Nucleophilic additions to carbonyls; Organolithium, Organomagnesium, Organozinc, Organocopper reagents (restricted to 1,4-addition) in synthesis,

Use of compounds of Mg, Li, Cu, B and Si in organic synthesis.

Concepts in multistep synthesis- retrosynthetic analysis, disconnections, synthons, synthetic equivalents, reactivity, umpolung, selectivity, Functional Group Interconversion,

Protecting groups: Protection and deprotection of hydroxy, carboxyl, carbonyl, carboxy amino groups and carbon-carbon multiple bonds; chemo- and regioselective protection and deprotection; illustration of protection and deprotection in synthesis.

One-group disconnections: Disconnections of alcohols, olefins, ketones

Two-group disconnections: β-hydroxy carbonyl compounds, α,β-Unsaturated carbonyl compounds, 1,3- and 1,5-dicarbonyl compounds

Illogical Two-group disconnections: α-hydroxy carbonyl compounds, 1,2-diols, Illogical electrophiles, 1,4-dicarbonyl compounds

Text Books/References:

1. Organic Synthesis: The Disconnection Approach by S. Warren: Wiley publications.
2. Organic Reaction Mechanism by V. K. Ahulwalia and R. K. Parashar: Narosa publications
3. Organic Chemistry by Clayden, Greeves, Warren and Wothers: Oxford University Press.
4. Heterocyclic Chemistry by T. L. Gilchrist, Pearson Education, 3rd Ed. 2007.
5. Modern Organic Synthesis-An Introduction by G. S. Zweifel and M. H. Nantz: W. H.
    a. Freeman and Company, 2006
6. Comprehensive Organic Synthesis by B. M. Trost and I. Fleming, , Pergamon Press, 1992.
7.

CHG6123: Applied Chemical Analysis (4 credits: 3-1-0)

Air Pollution Monitoring and Analysis

Classification of air pollution monitoring levels, air quality, standards and index, monitoring and analysis of selected air borne pollutants : SO_2, NO_x, SPM, VOC's, Pb, CO_2, POP's, Hg, carbon and ozone air pollution control devices Viz ESP's, scrubber technique etc. Atmospheric chemistry of acid rains, photochemical smog, greenhouse effect, global warming, ozone hole.

Soil and Water Pollution

Soil and water quality standards, monitoring and analysis of selected soil water contaminates: COD, pesticides, heavy metals, POP's, fluoride, cynide, nitrate, phosphate, oil & greese, Geobiochemical impact of municipal solid waste, steel plants efficient, domestic sewage. Control devices of water pollutants.

Food Analysis

A. Introduction to general Constituents of food, Proximate Constituents and their analysis, Additives-Introduction -Types -Study of preservatives colors and Antioxidants and method of estimation, adulteration -Introduction, Types, Test for adulterants.

B. Introduction standards composition and analysis of following foods : Wheat, Bread, Biscuits, Jam, Jelly, Honey, Milk, Ice Cream, Butter, Cheese, Milk powder, Oils and Fats, Tea, Coffee, Soft drinks, Alcoholic beverages, Cercal and pulses, Confectionery, Fruits, Vegetables, Egg, Fish, Meat.

Cosmetics, Clinical and Drug Analysis

A. Introduction of Cosmetics, evaluation of cosmetics materials, raw material and additives, Cosmetics colors, Perfumes in cosmetics, Cosmetics formulating, introduction, standards and methods of analysis, Creams, face powders, Make-up, Shaving preparations, Bath preparations.

B. Concepts and principles of analytic methods commonly used in the clinical species: i.e. ammonia, blood urea Nitrogen, Ca, Cl, CO_2, Fe, K, Li, Mg, Na, P, urea, glucose. Method for analysis of proteins (i.e. albumin, bilirubin, creatinine, cholesterol, HDL-cholesterol, triglycerides, creatinine) and Enzymes (i.e. Aanine Aminotransferase, acid phosphatase, alkaline phosphatase, amylase, aspartate aminotransferase, cholinesterase, lactate, and lipase).

Text Books/References:

1. Environmental Chemistry, S.E. Manahan, Lewis Publishers.
2. Environmental chemistry, Sharma and Kaur, Krishna Publishers.
3. Environmental Chemistry, A.K. De, Wiley Eastern.
4. Environmental Chemistry, Analysis, S.M. Khopkar, Wiley Eastern.
5. Standard Method of Chemical Analysis, F.J. Welcher Vol. III, Van Nostrand Reinhold Co.
6. Environmental Toxicology, Ed. J. Rose, Gordon and Breach Science Publication.
7. Environmental Chemistry, C. Baird, W.H. Freeman.
8. Analytical chemistry, G.D. Christian, J. Wiley.

9. Fundamentals of Analytical Chemistry, D.A. Skoog, D.m. West and F.J. Holler, W.B. Saunders.
10. Analytical Chemistry -Principles, J.H. Kennedy, W.Saunders.
11. Analytical Chemistry-Principles, and Techniques, L.G. hargis, Prentice Hall.
12. Principles of Instrumental Analysis, D.a. Skoog and J.L. Loary, W.B. Saunders.
13. Principles of Instrumental Analysis, D.A. Skoog, W.B. Saunders.
14. Quantitative Analysis, R.A. Day, Jr. and A.L. Underwood, Prentice Hall.
15. Environmental Solution Analysis, S.M. Khopkar, Wiley Eastern.

CHG6124: Solid State Chemistry (4 credits: 3-1-0)

Introduction, Crystal structure, Crystalline solids, Crystal systems, Metallic structure-Unit cells, Crystallographic directions and planes, linear and planar densities, close-packed crystal structures, Types of close packing-hcp and ccp, packing efficiency, Ceramics structure-radius ratio. Method of characterization-Powder X-ray diffraction, electron and Neutron diffraction, Thermal analysis, microscopic and spectroscopic techniques as tools for material characterization. Semiconducors - intrinsic and extrinsic, Hall Effect, Insulators-dielectric, ferroelectric, pyroelectric and Peizoelectric properties, Magnetic properties-Dia, para, ferro, ferri, antiferro and antiferri materials, Defects and dislocations-Vacancies and interstitials, dislocations and grain boundaries colour centers and reactivity, Amorphous materials-glasses and refractories, Superconductivity-Theory and its application.

Text Books/References:

1. C. Kittel, Introduction to Solid State Physics, 6th edition, Wiley, 1991.
2. A. R. West, Solid State Chemistry and Its Applications, Wiley, 1989.
3. Wells A. F. *Structural Inorganic Chemistry,* Oxford University.
4. Rao C. N. R. and Gopal Krishnan J. *New directions in solid state Chemistry*, Cambridge press.

1. P. A. Cox, Electronic Structure and Chemistry of Solids, Oxford University Press, 1991.
2. A. W. Adamson, Physical Chemistry of Surfaces, Wiley, 1990.
3. H. V. Keer, Principles of the Solid State, Wiley Eastern, 1993.
4. D. K. Chakrabarty, Solid State Chemistry, New Age International, 1996.
5. A. Zangwill, Physics at Surfaces, Oxford University Press, 1988.

CHG6125: Organic Chemistry Laboratory (6 credits: 0-0-12)

Elemental Analysis of Organic Compounds (C, H, N, O, S), Identification of organic compounds having at least two functional groups; Preparation of (a) p-Iodo tolune, (b) Benzaldehyde to Benzoin → Benzil → Benzilic acid, (c) Benzoic acid → o-Benzoyl Benozoic acid → Anthraquinone → Anthrone, (d) Ethylacetate → Ethylaceto acetate, I Anisole → Phenacetin; Synthesis of a simple dye and check, its purity by paper chromatography and extinction coefficient measurement; Estimation : (a) Methoxy group, (b) Acetyl group, (c) Nitrogen, (d) Carbon and hydrogen, Spectrophotometric analysis of Keto group

Text Books/References:

1. V. K.Ahluwalia and R. Aggarwal, Comprehensive practical organic chemistry, University press. 2000
2. B. S. Furniss, Vogel's Text Book of Practical Organic Chemistry, ELBS Longman, 5th Edition, 1996.
1. D. S. Gupta, Experimental Organic Chemistry, Qualitative and Quantitative, TATA MCGRAW HILL 2004
2. A. Ault, Techniques and Experiments for Organic Chemistry, University Science Book. 1998

4th Semester

List of Electives

CHG6126: Environmental Chemistry (4 credits: 3-1-0)

Chemistry of Environment: Environmental segments, atmospheric structure Chemistry of lower and upper atmosphere, radiation balance of earth .Major air pollutant, sources and their effect. Green house effect, acid rain, depletion of ozone layer, global warming. Air pollution abatement technology. Chemistry of water environment: Classification of water pollutants, characteristics of waste water, water quality parameters and their measurements. Waste water treatment: preliminary, primary, secondary, tertiary treatment. Waste water from some typical industries, sources, characteristics, effect and treatment option: textiles, refinery, leather, foods, sugar, fermentation, paper and pulp, fertilizer, soap and detergents, electroplating and pharmaceuticals. Solid waste disposal and management: classification and origin, methods of solid waste disposal. Microbiology involved in solid waste disposal. Soil pollution :Chemical composition of the soil, the exploitation of the mineral resources and abuse of the earth, soil pollution due to natural and artificial agencies and its effects, remedial measures to check the pollution. Energy and Environment: Energy sources, renewable and non-renewable, primary and secondary fossil fuels, their occurrence and estimation of reserves.

Text Books/References:

1. Mani Vasakam, Physico Chemical Examination of Water, Sewage and Industrial effluents, Pragati, 1991.
2. A. K. Dey, Environmental Chemistry, Wiley Eastern, 2002.
3. L.T. Pryde, Environmental Chemistry – An Introduction, Menlopark, 1973.
4. Environmental Chemistry: A Global Prospective, Oxford University, 2000

CHG6127: Supramolecular Chemistry (4 credits: 3-1-0)

From molecular to supramolecular chemistry: factors leading to strong binding, hydrogen bonding and stacking interactions. Molecular models of biological receptors, biomimetic chemistry, design, synthesis and binding studies of synthetic receptors. Metal guided self assembly reactions, molecular knot with double helical complexes of Cu (I). Self assembly of

polynuclear metal complexes. New molecular receptors: crown ethers, siderophores, cyclophanes, cyclodextrin and their application in specific recognition processes. Anion coordination chemistry and recognition. Supramolecular reactivity and catalysis, supramolecular devices.

Text Books/References:

1. J.W. Steed, J. L.Atwood , Supramolecular Chemistry, John Wiley, 2000.
2. H. W. Roesky, Rings, Clusters & Polymers of the main group & Transition Elements,Elsevier, 2003
3. P. Beer, P. Gale and D. Smith, Supramolecular Chemistry, Oxford Chemistry Primers.1999.
4. J. M. Lehn, Supramolecular Chemistry, VCH, New. York, 1973.

CHG6128: Industrial Chemistry (4 credits: 3-1-0)

Petrochemicals: Introduction. Classification of petrochemicals. Manufacture of some common petrochemicals.

Explosives: Characteristics of explosives, classification of explosives- primary & secondary explosives, preparation and application of some commercial explosives.

Cement: Types and composition of cements, raw material, manufacturing. Chemistry of setting of cement. Various additives used. Reinforced cement concrete. High performance concrete.

Dust Suppressant: Chemistry and source of dust. Dust suppressants. Paints and Pigment: Pigments-characterization and types, properties. Paints-classification, properties and applications of paints. Manufacture of paints.

Text Books/References:

1. Structural Methods in Inorganic Chemistry, E. A. V. Ebsworth, D. W. H. Rankin, & S. Cradock, 2nd Ed. 1991, CRC Press, Boca Raton, Florida,
2. Circular Dichroism: Principles and Applications, Nakanishi, K., Berova, N., Woody, R. W., Eds.; VCH Publishers, Inc.: New York, 1994.

CHG6129: Nanochemistry (4 credits: 3-1-0)

Introduction: size dependence on the properties of nanostructured materials -quantum confinement. Synthetic Methods: Top down and bottom up approaches. Chemical Routes and

Physical methods. Importance of nanoscale morphology. Techniques for characterization: BET method for surface area analysis, dynamic light scattering for particle size determination. One dimensional, two dimensional and three dimensional nanostructured materials, Quantum Dots, metal oxides, metal nanoparticles, semiconductors, core-shell structured nanocomposites. 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. Plasmon Resonances in Nanoparticles. Photocatalysis: 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 organic contaminants – environmental applications. Presentation by the student on assigned topic.

Text Books/References:

1. G. Ozoin, Nanochemistry: A Chemical approach to nanomaterials, Springer-Verlag, 2005.
2. C. N. R Rao, A. Muller, A. K Cheetham, Nanomaterials Chemistry, Wiley-VCH, 2007.
3. T. Pradeep, Nano: The Essentials, Tata McGraw-Hill, New Delhi, 2007.
4. G. Cao, Nanostructures and Nanomaterials – Synthesis, Properties and Applications, Imperial College Press, London, 2004, chapters 3, 4 and 5.
5. M. Hosokawa, K. Nogi, M. Naito, Y. Yokoyama, Nanoparticles Technology Handbook, Elsever

CHG6130: Corrosion Science and Techniques (4 credits: 3-1-0)

Definition of Corrosion & Stability of Metals

Theories of corrosion of metals and alloys [Local cell theory (Role of NMI), Micro galvanic cell (Structural heterogeneity); Differential Oxygen-concentration cell etc. Forms of Corrosion: Uniform corrosion, Localized corrosion, Pitting corrosion, Erosion corrosion, Fretting corrosion, Cavitational damages, Crevice corrosion; Selective leaching; Graphitisation; Dezincification; Ring worm attack; Galvanic corrosion; Filliform corrosion; Exfoliation; Intergranular attack; Weld decay; Knife line attack; Stress Corrosion Cracking (SCC); Caustic embrittlement;, Hydrogen Assessed Cracking (HAC); Corrosion fatigue; Fretting corrosion; Fretting fatigue; Liquid metal embrittlement (LME);Weldment corrosion;

Marine & Underground corrosion; Stray current attack; In vivo corrosion; Metal matrix composite (MMC) corrosion; Microbial (S.R.B.) corrosion of steel in concrete.

Factors affecting corrosion and Prevention Techniques

Environments; Temperature, Turbulence, Concentration-gradient, pH; Once-through & closed re-circulating cooling water system; State of stress, etc.

Text Books/References:

1. M.G. Fontana & Greene, Corrosion Engineering; Tata McGraw Hill
2. L.L. Shrier (Vol. I & II), Corrosion & corrosion control.

CHG6131: Computational Chemistry (4 credits: 3-1-0)

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

Text Books/References:

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

CHG6132: Polymer Chemistry (4 credits: 3-1-0)

Introductory concepts, definition, common system chemistry and classification of polymers, synthetic and natural polymers, types of polymerization, addition, condensation, co-ordination and ring opening polymerization, Preparation, properties and uses of some important thermoplastic (i.e. PE, PVC, Teflon, PS, PMMA)and thermosetting resins (i.e. Phenolic resin, Amino resin and Epoxy resin), natural and synthetic rubbers, Fibers

(i.e. Nylons, PAN, Polyurethanes). Polymer Characterization: molecular weight studies and molecular weight distribution, polydispersive index, determination of molecular weight of polymers. Polymer behaviour, crystalline and thermal behaviour, Glass transition temperature, factor influencing glass transition. Polymerization techniques: bulk, solution, emulsion, and suspension polymerization, polymer colloids and polymer solution. Thermodynamics aspect of Polymerization, Stereo Chemistry and mechanism of polymerization: free radical, cationic and anionic polymerization. Relevant aspects of physical properties of polymer systems, rheological properties, polymer processing, processing techniques i.e. molding, casting, extrusion and, calendaring techniques. Polymer degradation and stabilization, biological degradation of polymers. environmental pollution by polymers.

Text Books/References:

1. J. W. Nicolson, The chemistry of polymers, RSC publishing, 3rd Ed., 2006
2. P. Bahadur and N.V. Sastry, Principles of Polymer science, Norosa Publication, 2nd Edition, 2005.
3. F. W Billmeyer, Text book of Polymer Science, Johns Wiley and sons Publication, 3rd Edition, 1984
4. M. Cambell, Introduction to synthetic polymer, Oxford university press, 2nd Ed., 2000.

CHG6133: Nuclear Chemistry (4 credits: 3-1-0)

Radioactive Decay Processes: Alpha decay- penetration of potential barriers, Hindered alpha decay, Alpha decay energies; Beta decay- Fermi theory, Kurie plots, comparative half-lives, Electron capture, Selection rules, Forbidden transitions, Non-consertation of parity, neutrinos; Gamma decay- half-life of excited states, Multipole radiation and selection rules, isomeric transition, internal conversion and Auger effect.

Nuclear Structure: Nuclear stability and binding energy. Mass and binding energy systematics, semi-empirical binding energy equation. Nuclear isomerism and internal conversion; Nuclear volume and density; Nuclear forces; Nuclear energy levels; Nuclear models; Liquid drop, Shell and Fermi gas models, Elementary ideas about Collective model.

Nuclear Reactions and Nuclear Energy: Nuclear reactions; Nuclear fission and cross-section, Chain fission, Fission product and fission yield, Mass and charge distribution in

fission; Compound nucleus formation & Q-values; Methods for production of some most commonly used radiotracers(^{3}H, ^{14}C, ^{32}P, ^{35}S, ^{131}I); Labelling; Nuclear fission; Chain reactions; Nuclear reactors; classification & Fermi's 4-factor formula; Reprocessing of used fuel rods; Production of transurides and transcurides by successive neutron capture in a nuclear reactor; Heavy ion induced nuclear reactions – Production of super Heavy Elements (SHE); Nuclear fusion

Nuclear Processes in Geology, Geochemistry & Astrophysics: Ages of Rocks and Minerals; Age of earth-Radioactive dating; nuclear fusions reactions, threshold, Nuclear reactions in stars and Nucleogenesis; Nuclear fusion and stellar energy (Cosmo chemistry).

Text Books/References:

1. H. J. Arnikar, Essentials of Nuclear chemistry, 4th Ed., Wiley-Eastern Ltd. New Delhi
2. G. Friedlander, J. W. Kennedy, E. S. Macias and J. M. Miller, Nuclear and Radiochemistry, 3rd Ed., John-Wiley & Sons, New York
3. B. G. Harvey, Introduction to Nuclear Physics and Chemistry, Prentice Hall.
4. K.S. Krane, Introductory Nuclear Physics, Wiley India, ISBN No.:978-265-1785-5
5. M. Haissinsky, Nuclear Chemistry & Its Applications, Addison-wisley.
6. M. Lefart, Nuclear Chemistry, Von Nostrand.
7. G. T. Seabag, Man Made Transuranium Elements.
8. A. N. Nesmeyanov, Radiochemistry, Mir Publishers, Moscow.

CHG6134: Natural Products (4 credits: 3-1-0)

Introduction to natural products and metabolites.

Terpenoids: Introduction, isolation and classification of terpenoids; general properties, structure determination and synthesis of Citral, Geraniol, Linalool, Menthol, α-Pinene, Camphene, Camphor, Abietic acid, Squalene, Taxol, Rubber, Carotenoids and Vitamine A,

Steroids: Introduction, nomenclature of steroids, stereochemistry and absolute configuration of steroid; occurrence, isolation, structure elucidation, and chemical properties of Cholesterol; synthesis and bio-synthesis of cholesterol; Bile acids; Androgens, Testosteron, Oestrons, Cortisone; Vitamine D.

Alkaloids: Introduction, occurrence and isolation, function of alkaloids in plant, general properties, nomenclature, and classification of alkaloids, isolation, properties and structural elucidation of Quinine, Morphine, Nicotine, Lysergic acid, Caffeine, Strychnine and Reserpine.

Prostaglandins: Introduction, nomenclature, Approaches to prostaglandin E and F synthesis.

Vitamins and Harmones: Introduction, chemical properties and structure elucidation of Vitamins A, B, C and Vitamin D; and Hormones: Androgens, Testosteron, Oestrons, Cortisone.

Text Books/References:

1. I. L. Finar, Organic Chemistry, Vol II. ELBS and Longman Ltd., New Delhi.
2. S. V. Bhat, B. A. Nagaramgagi, M. Srikumar, Chemistry of Natural Products, Alpha Science International Ltd, 2005.
3. O. P. Agarwal, Chemistry of Natural Products, Vol- 1 &Vol-2, Goel publishing House, 1989.
4. K. C. Nicolaou, T. Montagnon, Molecules that Changed World, Wiley-VCH, 2008.
5. J. W. Apsimon, Total Synthesis of Natural Products, Vol. 1-6, Wiley Interscience.
6. J S Bindra and R. Bindra, Prostaglandin Synthesis, Academic Press Inc., 1977.
7. K. C. Nicolaou, Classics in Total Synthesis of Natural Products, Vols. 1 and II.

CHG6135: Methods in Organic Synthesis (4 credits: 3-1-0)

Reaction vs synthetic method; metal atom functionality in organometallic reactions, organometallics as protecting and stabilizing groups, palladium catalyzed reactions, Heck reaction, cross coupling reactions (Suzuki, Stille, Negishi, Kumada, Hiyama, Sonogashira, Buchwald-Hartwig), Fischer carbenes, Schrock carbenes, Olefin metathesis, various types of metathesis and application to organic synthesis, Dotz benzoannulation, Pauson-Khand reaction, [2+2+2] cycloadditions, Grignard reactions, Rieke magnesium, 1,2 vs 1, 4-addition, cerium reagents, copper reagents, homocuprates, lower order cuprates, higher order cuprates, chromium arene complexes and reactions, McMurry coupling, role of silicon in organic synthesis, origin and consequence of alpha effect and beta effect involving silicon compounds, role of silicon in few name reactions. Some selected natural and non-natural

product synthesis involving these reactions. Concise introduction to asymmetric synthesis, detailed discussion on resolution, chiral auxiliaries, chiral ligands, chiral catalysts and organocatalysts with specific examples.Introduction to domino/tandem/cascade reaction concepts with selected examples

Text Books/References:

1. G. S. Zweifel and M. H. Nantz, Modern Organic Synthesis-An Introduction, W. H. Freeman and Company, 2006.
2. B. M. Trost and I Fleming, Comprehensive organic synthesis, Pergamon Press, 1992.
3. Organanometallics in Organic Synthesis, J. M. Swan, D. St. C. Black, Chapman and Hall, London, 1974
4. Organotransition Metal Chemistry: Applications to Organic Synthesis, S. G. Davis, Pergamon Press, Oxford, 1982.
5. Basic Organometallic Chemistry, B. D. Gupta, A J Elias, Universities Press, Chennai, 2010
6. Transition Metals in the total synthesis of complex organic molecules, L. S. Hegedus, University Science Books, 1994.

CHG6136: Surface Chemistry (4 credits: 3-1-0)

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.

Text Books/References:

1. P. W. Atkins, Physical Chemistry, 6thEdn., Oxford University Press, 1998.

2. D. McQuarie, and J. D. Simmen, Physical Chemistry, 1stEdn., 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 - Mukerjee, Fundamentals of Photochemistry, Wiley 1992.

7. P. K. Ghosh, Introduction to Photoelectron Spectroscopy, Wiley Interscience, 1983.

CHG6137: Photochemistry and Its Applications (4 credits: 3-1-0)

Principles and concepts: An overview of: Laws of photochemistry, Beer-Lambert law, electronic energy levels, atomic and molecular term symbols, singlet-triplet state, intensity and strength of electronic transition, selection rules for electronic transition, Jablonski diagram and photophysical processes, Franck-Condon principle. Excited state lifetime, steady state and time resolved emission, factors affecting excited state energy: solvent effect on spectra-non-specific and specific interaction (H-bonding and charge transfer), Characteristics of CT interaction. Apparent violation of selection rule (Vibronic coupling and spin orbit coupling)

Excited state kinetics, quantum yield expressions, excimer and exciplex, kinetics of luminescence quenching: static and dynamic, Stern-Volmer analysis, deviation from Stern-Volmer kinetics. Photoinduced electron transfer rates, free energy dependence of electron transfer on rate, Photoinduced energy transfer, FRET, rate and efficiency calculation of FRET.

Methods: Measurement of fluorescence and phosphorescence and lifetimes. Introduction to time-resolved techniques for absorption and emission measurements, detection and kinetics of reactive intermediates. Examples of low temperature matrix isolation of reactive intermediates.

Reactions: Photochemistry of alkene, cis-trans isomerization, photocycloaddition reactions of alkene, photochemical electrocyclic and sigmatropic reactions, di-pi-methane rearrangment, electron transfer mediated reactions of alkene. Photochemistry of carbonyl compounds, Norrish type I and type II reactions, enone and dienone cycloadditions. Photochemistry of aromatic systems, electron transfer and nucleophilic substitution reactions. Photochemistry of

nitro, azo and diazo compounds. Photochemistry involving molecular oxygen, generation and reactions of singlet oxygen. Photo-fragmentation reactions (Barton, Hofmann-Loffler-Freytag)

Applications

Fluorescence based sensors – examples of molecular and supramolecular systems. Conversion of solar energy to chemical and other forms of energies, solar photovoltaic cell, basic principle and design of the cell. Excited state pKa of phenols.

Text Books/References:

1. *Fundamental of Photochemistry*, K. K. Rohatgi-Mukherjee, New Age International (P) Ltd., New Delhi, 1986.
2. *Principles of Fluorescence Spectroscopy*, 3rd Ed., J. R. Lakowicz, Springer, New York, 2006.
3. *Fundamentals of Photoinduced Electron Transfer*, G. J. Kavarnos, VCH publishers Inc., New York, 1993.
4. *Molecular Fluorescence: Principles and Applications*, B. Valeur, Wiley-VCH Verlag GmbH, Weinheim, 2002.
5. *Modern Molecular Photochemistry of Organic Molecules*, N. J. Turro, V. Ramamurthy, J. C. Scaiano, University Science, Books, CA, 2010.

CHG6138: Advanced Quantum Mechanics (4 credits: 3-1-0)

Elementary ideas of vectors, Matrices, n-dimensional vector space, matrix representation of operators, Hermitian operators, Hermitian matrices, Commutability and compatibility, Heisenberg Uncertainty principles (Operator methods), Heisenberg's equation of motion, constant of motion, virial theorem, Parity, time reversal symmetry. Angualr momentum operator-commutation relation-step up and step down operator in polar coordinates. Projection operators and their properties-projection operator techniques and angular momentum. Rotational groups and angular momentum operator.

Hydrogen like systems, complete wave equation, radial and angular plots, hydrogen spectra, spin angular momentum, hydrogen like wave functions. Many electron atom (He), approximation methods: independent particle method, perturbation method (treatment of ground state of He atom), variation method (treatment of ground state of He atom),

self consistent field approximation, Slater type orbitals, Symmetric and antisymmetric wave functions, Pauli's exclusion principle, vector model of atom; spin orbit coupling, spectroscopic term symbols for atomsRussel- Saunder's terms and coupling schemes- ntroduction to SCF methods- Hartree and Hartree-Fock's SCF Polyatomic basis sets, Gaussian, double-zeta and polarized basis sets, population analysis and dipole moments. The Thomas-Fermi model of the atom.

The metallic bond. Bloch theory, free electron and tight binding model. Effective crystal field Hamiltonian: Steven's equivalent operator method.

Hohenberg-Khon theorem and elements of Density function theorem.

Text Books/References:

1. Nouredine Zettili, Quantum Mechanics (Concept and Applications) 2nd Edition.
2. G. Arfken and Hans J. Weber, Mathematical methods for physicists.
3. I. N. Levine, Quantum Chemistry, 3rd edition.
4. D. J. Griffiths, Introduction to Quantum Mechanics, 2nd Edition.
5. Rbert Eisberg and Robert Resnik. Quantum Physics of Atoms, Mlecules Solids, Nuclei and Particles, 2nd Edition.
6. John Powel and Bernd Crasemann, Quantum Mechanics

CHG6139: Advanced Magnetic Materials (4 credits: 3-1-0)

Magnetism: Fundamentals and Theory, Magnetic fields, Magnetization and magnetic moments, magnetic measurements. Single molecule magnet and their properties Magnetic materials: Classifications of Magnetic Materials, Magnetic properties, Hysteresis and related properties, Parametric characterization of hysteresis, Cause of hysteresis, Micromagnetism, Magnetic order and critical phenomena, Theories of paramagnetism and diamagnetism, Novel Techniques for Characterizing and Preparing Samples , Novel Materials, Spintronics and Magnetoelectonics. Magnetics-technological applications: Soft magnetic materials, Hard magnetic materials, Magnetic recording, Magnetic evaluation of materials.

Text/ Reference Books:

1. Jiles D. *Introduction to Magnetism and Magnetic Materials*, Taylor and Francis.

2. Kronmüller H. and Parkin S. *Handbook of Magnetism and Advanced Magnetic Materials*, Wiley.