Proposed Syllabi for CST B.Tech. Curriculum

CH 101: Chemistry (3-1-0-8)

Structure and Bonding; Origin of quantum theory, postulates of quantum mechanics; Schrodinger wave equation: operators and observables, superposition theorem and expectation values, solutions for particle in a box, harmonic oscillator, rigid rotator, hydrogen atom; Valence Bond and Molecular Orbital Theories; Hydrogen Molecule; Hybridization; Molecular Symmetry; Electronic Spectroscopy and Lasers. Chemical Thermodynamics and Chemical Kinetics.

Coordination compounds: ligand, stereochemistry, crystal field and molecular orbital theories; Bioinorganic chemistry and organometallic chemistry; Chemistry of materials.

Stereochemistry of more than two stereo-centers, R&S and E&Z nomenclature, Conformation of cyclohexane and 1,2-disubstituted cyclohexane; Pericyclic reactions; Bioorganic chemistry: proteins, enzymes, carbohydrates, nucleic acids and lipids; Natural products: classification and origin of terpenoids, alkaloids and steroids. Macromolecules (polymers); Solid phase synthesis; Green chemical processes. Modern spectroscopic techniques in structural elucidation of organic compounds (UV-vis, IR, NMR).

Books:

1. P. W. Atkins, *Physical Chemistry*, 5th Ed., ELBS.
2. C. N. Banwell, and E. M. McCash, *Fundamentals of Molecular Spectroscopy*, 4th Ed., Tata McGraw-Hill.
3. F. A. Cotton, and G. Wilkinson, *Advanced Inorganic Chemistry*, 5rd Ed., Wiley.
4. D. J. Shriver, P. W. Atkins, and C. H. Langford, *Inorganic Chemistry*, 3rd Ed., ELBS.
5. S. H. Pine, *Organic Chemistry*, McGraw-Hill, 5th Ed.

References:

1. I. A. Levine, *Physical Chemistry*, 4th Ed., McGraw-Hill.
2. I. A. Levine, *Quantum Chemistry*, EE Ed., Prentice Hall.
3. G. M. Barrow, *Introduction to Molecular Spectroscopy*, International Edition, McGraw-Hill.
4. J. E. Huheey, E. A. Keiter and R. L. Keiter, *Inorganic Chemistry: Principle, structure and reactivity*, 4th Ed., Harper Collins.

5. L. G. Wade (Jr.), *Organic Chemistry*, Prentice Hall.

CH 212 Inorganic Chemistry (3-0-0-6)

Acids and bases: classification, Lewis acid and base concept, hard acid, hard base classification, Pearson's HSAB concept and application; Oxidation and reduction: redox reactions, redox potential, electrochemical series, use of electrochemical series; Metallic chains, sheets and clusters; Metal silicates, zeolites and polyoxo-metallates; Metals and alloys, ceramic materials, intermetallic compounds and zintl phases; Chemistry of phosphorus, phosphorus oxides and phosphorus hydrides; Chemistry of oxyacids and oxyanion of nitrogen and phosphorus; Differences between the chemistry of nitrogen and phosphorus; Chemistry of the halogens: pseudo-halogen, inter-halogen; Oxides and oxyacids; Polyhalides; Chemistry of the rare gases: Chemistry of xenon, structure and bonding of xenon compounds; Non-aqueous solvents: types of solvents, general characteristics, reactions in non-aqueous solvents with reference to liquid NH3 and liquid SO2.

Text Books:

1. N. N. Greenwood and A. Earnshaw, Chemistry of the Elements, 2nd Ed., London: Butterworth Heinmann ,1997.

2. D. J. Shriver, P. W. Atkins and C. H. Langford, Inorganic Chemistry, 2nd Ed., Oxford ,1994.

References:

1. F. A. Cotton and G. W. Wilkinson, Advanced Inorganic Chemistry, 5th Ed., John-Wiley & Sons, 1988.
2. J. E. Huheey, E. A. Keiter and R. L. Keiter, Inorganic Chemistry: Principles of Structure and Reactivity, Dorling Kindersley, 2006.
3. P. K. Dutt, Concepts of Chemistry, Levant Book, 2004.

CH 221 Organic Chemistry (3-1-0-8)

Introduction to types of organic reactions; Structure and stability of reactive intermediates: carbocations, carbanions, free radicals, carbenes, arynes and nitrenes; Methods of determining organic reaction mechanism: thermodynamic and kinetic requirements, transition state theory, Hammond postulate, Curtin-Hammett principle, kinetic vs. thermodynamic control reaction, isotope effects, substituent effects, Hammett linear free energy relationship, Taft equation; Addition reaction to C=C and C=O; Preliminary idea of radical reactions; Application of Oxidation and Reduction reactions and reagents, Name reactions (e.g. Sharpless epoxidation, Suzuki coupling, Heck coupling etc.). Mechanism of aromatic nucleophilic and electrophilic substitions; Introduction to synthesis of nucleic acids and peptide chemistry.

Texts:

1. E. V. Anslyn and D. A. Dougherty, *Modern Physical Organic Chemistry*, 1st Ed., University Science Books, California ,2006.
2. F. A. Carey and R. J. Sundberg, *Advanced Organic Chemistry: Structure and Mechanisms (Part A and B),* Kluwer Academic/ Plenum Pub., 2000

References:

1. P. Sykes, *A guide to mechanism in Organic Chemistry*, 6th Ed., Pearson Education, 2004.
2. M. B. Smith and J. March, *Advanced Organic Chemistry*, 6th Ed.., John Wiley and Sons, Inc, 2007.
3. D. Nasipuri, *Stereochemistry of Organic Compounds*, Wiley, 1994.

CH 231 Introduction to Quantum Chemistry (3-0-0-6)

The motivation for Quantum mechanics: Historical background, postulates and general principles of quantum mechanics; Operators and their properties; Schrödinger equation, its application on some model systems : free-particle and particle in a box (1D and 3D), tunneling, the harmonic oscillator, the rigid rotator, and the hydrogen atom; Approximate methods; The variation theorem; Linear variation principle; Perturbation theory; Applications of variationalmethods and perturbation theory to the helium atom; Angular

momentum: Eigenfunctions and eigenvalues of angular momentum operator, Ladder operator, addition of angular momenta; Spin- Pauli Exclusion Principle; Slater determinants; Term symbol (RS and jj coupling) and spectroscopic states, spin-orbit coupling and Zeeman splitting; Virial theorem; Born-Oppenheimer approximation; VB and MO theory, Application to H_2^+, H_2 molecule; Hückel molecular orbital theory and its application to ethylene, butadiene and benzene; Hybridization and valence MOs of some simple molecules.

Texts:

1. P. W. Atkins and R. S. Friedman, *Molecular Quantum Mechanics*, 3rd Ed., Oxford University Press,1997.
2. D. A. McQuarrie, *Quantum Chemistry*, Viva Books, 2003

References:

1. I. N. Levine, *Quantum Chemistry*, Prentice Hall, 2003
2. F. L. Pilar, *Elementary Quantum Chemistry*, 2nd Ed., Dover Publications, Inc. NY, 1990.

CH 222 Applied Organic Chemistry (3-0-0-6)

Fats, Oils and detergents: Natural fats, edible and industrial oils of vegetable origin, common fatty acids, glycerides, hydrogenation of unsaturated oils, soaps, synthetic detergents, alkyl and aryl sulphonates; Synthetic polymers: polymerization, methods of polymerization, step growth polymerization, structure and physical properties, natural and synthetic rubbers; Synthetic dyes: Color and constitution (electronic concept), classification of dyes, synthesis of methyl orange, congo red, malachite green, crystal violet, phenolphthalein, fluorecein, alizarin and Indigo; Fuels and sources of Energy: Chemical fuels, classification of fuels, characteristic of fuel, calorific value and its determination, petroleum, cracking, reforming of petrol, knocking, antiknocking agent, diesel engine fuel, octane number, synthetic petrol, biodiesel; Liquid Crystals: Liquid crystal phase, classification of liquid crystals, chemical constitution and liquid crystalline behavior, molecular structure and liquid crystals, application of liquid crystal.

Texts:

1. R. T. Morrison and R. N. Boyd, *Organic Chemistry*, 6th Ed., Prentice–Hall, 2004.

2. B. Billmeyer, *Text book of Polymer Science,* 3rd Ed., John Wiley & Sons, 1984.

References:

1. I. L. Finar, *Organic Chemistry, Vols. 1 and 2*, 5th Ed., Pearson education, 2005.
2. D. Singh, B. Deshwal and S. K. Vats, *Comprehensive Engineering Chemistry,* I. K. International, Mumbai, 2007.
3. R. V. Gadag and A. N. Shetty, *Engineering Chemistry*, I. K. International, 2006.
4. M. P. Stevens, *Polymer Chemistry,* 3rd Ed., Oxford University Press Inc., 1998.

CH xyz: Group Theory (3-0-0-6)

Definitions and Theorems of Group Theory: Properties of Group and examples, Subgroups, Classes. Molecular Symmetry and the Symmetry Groups: Symmetry elements and Operations: symmetry planes and reflections, the inversion Center, Proper Axes and proper rotation, and Improper axes and improper rotations. Products of symmetry Operations. Equivalent symmetry elements and equivalent Atoms. General relations among symmetry elements and Operations. Symmetry Elements and Optical Isomerism. The symmetry point groups. Symmetries with multiple High- Order Axes. Classes of symmetry Operations. A systematic Procedure for symmetry Classification of molecules. Representations of Groups: Comments on Matrices and Vectors. Representation of groups. The "Great Orthogonality Theorem" and its consequences. Character Tables. Representation for Cyclic Groups. Group Theory and Quantum Mechanics: Wave function as bases for irreducible representations. The Direct Product. Detection of non–zero integrals. Symmetry Adapted Linear Combinations: Derivation of Projection Operators. Use of Projection Operators to construct SALCs. Molecular Orbital Theory and its Application in Organic Chemistry: General Remarks. Symmetry factoring of secular equations. Carbocyclic system. More general cases of LCAO-MO bonding. Naphthalene. Electronic excitations of Naphthalene:selection rules and configuration interaction. Three center Bonding. Symmetry based selection rules for cyclization reactions. Molecular Orbital Theory for Inorganic and Organometallic Compounds: Transformation Properties of Atomic Orbitals. Molecular orbitals for bonding in ABn molecules: The Tetrahedral AB4 cases. Molecular orbitals for bonding in ABn molecules.

Text Book

1. F. A. Cotton, Chemical Applications of Group Theory, 3rd Ed, John Wiley & Sons, 1990.

Reference:

1. Molecular Symmetry and Group Theory: A Programmed Introduction to Chemical Applications" by Alan Vincent; 2nd Edition, Wiley.

CH 211 Industrial Chemistry (3-0-0-6)

Hydrazine: Manufacturing of hydrazine, Raschig process, Urea process, Bayer process, H_2O_2 process; Use of hydrazine as rocket fuel, in fuel cell; Insecticides and Herbicides: Definition and classification of Insecticides; Manufacturing of insecticides;Environmental effects; Definition and classification of Herbicides, Health effect; Mineral Fertilizers; Economic Importance, Manufacturing of N and P-containing Fertilizers; Construction Materials: Lime, Quicklime, Slaked Lime; Cement, Miscellaneous cement types, Composition and manufacturing of cements; Enamel: Classification, Enameling, Coating processes, Stoving of enamels; Ceramics: General Information and Classification, Physical: Chemical Processes related to manufacturing of clay ceramics, Metal and Metalloid ceramic materials; Metallic hard materials and fibers; Inorganic Pigments General information and Economic Importance, White pigments, Titanium Dioxide Pigments, Manufacturing processes for TiO_2 pigments, Applications for TiO_2 pigments, Lithopone and Zinc Sulfide pigments, Iron Oxide pigments, Chromium(III) Oxide Pigments, Magnetic Pigments, Manufacture of magnetic Pigments.

Text Books:

1. A. Heaton, *An introduction to Industrial Chemistry*, 3rd Ed., Blackie Academic, 1996.
2. K. H. Davis and F. S. Berner, *Handbook of Industrial Chemistry, Vols. 1 and 2*, CBS, New Delhi, 2005.

References:

1. T.W. Swaddle, *Inorganic Chemistry: An Industrial and Environmental Perspective*, Academic Press, San Diego, 1997.
2. K. Weissermel and H.J. Arpe, *Industrial Organic Chemistry*, 2nd Ed., Weinheim, VCH, 1996.

CH 233 Spectroscopic Techniques in Chemistry (3-0-0-6)

Region of spectrum, spectral lines intensity and broadening, Microwave spectrum of rigid and non-rigid rotator, Principle of microwave oven; Vibrationalspectra of harmonic and unharmonic oscillator, breakdown of Born-Oppenheimer approximation; Vibrations of polyatomic molecules, group frequencies and its applications; Raman spectra, structure determination; Electronic spectra of diatomic and poly atomic molecules; Photochemistry of vision, radiative and nonradiative decay, Lasers and its applications; Photoelectron spectroscopy; Spin resonance spectroscopy; Magnetic resonance imaging (MRI).

Texts:

1. C. N. Banwell and E. M. McCash, *Fundamentals of Molecular Spectroscopy*, Tata McGraw Hill, 1994.
2. P. Atkins and J. de Paula, *Atkins' Physical Chemistry* 7th Ed. Third impression, Oxford University Press, 2005.

References:

1. G. M. Barrow, *Introduction to Molecular Spectroscopy*, McGraw Hill, 1962.
2. H. E. White, *Introduction to Atomic Spectra*, McGraw Hill, 1934.
3. N. J. Turro, *Modern Molecular Photochemistry*, University Science, 1991.
4. B. Valeur, *Molecular Fluorescence Principles and Applications*, Wiley-VCH, 5th Reprint, 2009.

CH 223 Chemical Technology Lab - I (0-0-6-6)

Identification of unknown organic compounds: element detection, confirmation of the functional groups, derivatization; Separation technique: normal and reduced pressure distillation, solubility method, column chromatography method, sublimation; Isolation of medicinal compounds from plants/other sources: soxhlet extraction; Preparation: aspirin, paracetamol, imidazole, dye preparation; multistep synthesis; Estimation of organic compounds: paracetamol, glucose; Characterization of unknown organic compounds by UV-Vis, IR and ^{1}H-NMR techniques; Experiment based on polymer science, electrophoresis, protein estimation, catalytic hydrogenation.

Texts and References:

1. J. R. Mohrig, T. C. Morrill, C. N. Hammond and D.C. Neckers, *Experimental organic chemistry*, W.H. Freeman and Co. ,1998.
2. N. K. Vishnoi, *Advanced practical organic chemistry*, Vikash publishing house Pvt. Ltd. ,1996.
3. B. S. Furniss, A.J. Hannaford, P.W.G. Smith, and A.R. Tatchell, *Vogel's textbooks of practical organic chemistry*, 5th Ed., ELBS Longman ,1994.

CH 301 Environmental Chemistry (3-0-0-6)

Atmospheric composition and behavior; Principles of contaminant behavior in the environment; Chemistry in aqueous media; Chemical and physical reactions in the water environment; Major contaminant groups and their natural pathways for removal from water, Soil: Groundwater and subsurface contamination, Soil profiles, Acid-base and ion exchange reactions in soils, Fertilizers, wastes and pollutants in soil; Atmosphere and atmospheric chemistry: Inorganic and organic air pollutants, Sulfur dioxide sources and the sulfur cycle, Nitrogen oxides in the atmosphere, Smog forming reactions of organic compounds in the atmosphere, Mechanisms of smog formation; Nature and importance of chemical analysis: Major categories of chemical analysis, Application of analytical chemistry to environmental chemical analysis.

Texts:

1. S. Krause, H. M. Clark, J. P. Ferris, R. L. Strong, *Chemistry of the Environment*. Elsevier Science & Technology Books, 2002.
2. S.E. Manahan, *Fundamentals of Environmental Chemistry,* CRC Press, 2001.

References:

1. P. Patnaik, *A Comprehensive Guide to the Hazardous Properties of Chemical Substances,* John Wiley and Sons, Inc., 2007.
2. E. R. Weiner, *Applications of Environmental Chemistry: A Practical Guide for Environmental Professionals,* CRC Press., 2000.

CH 302 Technical Report and Presentation (0-0-3-3)

This course will addresses the technical report writing skills, basic communication skills, power point presentation and group discussions; Each student will required to prepare and

submit one typewritten bound copy of seminar paper on a selected technological topic related to the course / subject under the supervision of a faculty member; The student will deliver a talk based on the report with the help of power point presentation; The attendance in the seminar is compulsory for all the students.

Reference:

1. W. S. Pfeiffer, *Technical writing: A practical approach*, 2nd Ed., Prentice Hall, 1994.

CH 314 Chemical Technology Lab - II (0-0-6-6)

Modern synthetic and analytical techniques to synthesize and characterize industrially important inorganic compounds; Use of electro-inorganic synthesis, photosynthesis and nano-material synthesis for the preparation of inorganic materials; Synthesis and characterization of alum, phosphate fertilizers, soaps and detergents, superconductors and nano-matertials; Environmental inorganic chemistry: preparation of clathrate compounds and applications in catalysis.

Texts/References:

1. G. Svehla, *Vogel's qualitative inorganic analysis*, 7th Ed., Pearson Education, New Delhi, 2006.
2. J. Mendham, R. C. Denney, J. D. Barnes and M. J. K. Thomas, *Vogel's textbook of quantitative chemical analysis*, 6th Ed., Pearson Education, New Delhi, 2005.
3. A. J. Elias, *A Collection of Interesting General Chemistry Experiments*, Revised Ed., Universities Press (India) Pvt. Ltd, 2007.
4. K. Hutchings, *Classic Chemistry Experiments*, The Royal Society of Chemistry, London, 2000

CH 316 Frontiers of Coordination Chemistry (3-0-0-6)

Bonding: Molecular Orbital Theory, pi-bonding; Crystal field theory; Jahn-Teller effect; Spectrochemical series, nephelauxetic series; 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; Reaction Mechanism: Substitution in octahedral and square planar complexes; Lability, trans-effect,

Conjugate base mechanism; Racemisation; Electron Transfer Reactions: inner sphere and outer sphere mechanism; Marcus theory; Inorganic photochemistry: Photosubstitution and photoredox reactions of chromium, cobalt and ruthenium compounds; Adamson's rules; Lanthanides and Actinides: Spectral and Magnetic Properties; NMR Shift reagents; Coordination polymers and metal organic frameworks as storage materials, optoelectronic devices, magnetic materials; Polyoxometallates: structures, properties and industrial applications.

Text Books:

1. J. E. Huheey, E. A. Keiter and R. L. Keiter, Inorganic Chemistry: Principles of Structure and Reactivity; 4th Ed., Harper Collins, 1993.
2. B. E. Douglas, D. H. McDaniel and J. J. Alexander, Concepts and Models of Inorganic Chemistry; 3rd Ed., John Wiley, 1993.

References:

1. R. R. Jordan, Reaction Mechanism in Inorganic Chemistry; 2nd Ed., Oxford University Press, 1998.
2. J. Barrett, Inorganic chemistry in aqueous solution; Royal Society of Cambridge, 2004.

CH 331 Chemical Kinetics and Electrochemistry (3-0-0-6)

Rates of Chemical reactions: Elementary rate laws, temperature dependence of rate, opposing reactions, consecutive reactions, parallel reactions; Reaction mechanism, unimolecular reactions, reversible reactions; Relaxation method; Principle of microscopic reversibility; Complex reactions: chain reactions, branched chain reactions, polymerization reactions, catalysis, autocatalysis, enzyme catalysis; Theories of chemical kinetics: Collision theory, activated complex theory; Ionic reactions, kinetic salt effect; Adsorption and surface catalysis; Photochemistry: rates of photochemical processes, complex photochemical processes; Photosynthesis; Equilibrium Electrochemistry: Electrochemical cells, cell representation, types of electrodes, half reactions, standard potentials, types of electrochemical cells, cell reactions, cell EMF; Activity and activity coefficients;

Debye Huckel theory; Applications of standard potentials: electrochemical series, determination of activity coefficient; pH, pKa, solubility product; thermodynamic functions; Batteries and Fuel cells; Over potential; Mechanism of electrode reactions; Corrosion.

Texts:

1. K. Laidler, *Chemical Kinetics*, 3rd Ed., Pearson Education, 2004.
2. G. M. Barrow, *Physical Chemistry*, 5th Ed., Tata Mcgraw-Hill, 1992.

References:

1. R. J. Silbey and R. A. Alberty, *Physical Chemistry*, 3rd Ed., John Wiley & Sons,2002.
2. P. Atkins and J. de Paula, *Atkin's Physical Chemistry*, 7th Ed., Oxford University Press, 2002.
3. T. Engel and P. Reid, *Physical Chemistry*, 1st Ed., Pearson Education, 2006.
4. G. W. Castellan, *Physical Chemistry*, 3rd Ed., Narosa Publishing House, 1985.

CH 332: Computational Chemistry (3-0-0-6)

Computer programming in FORTRAN; Locating roots of equations; Numerical differentiation and integration; Systems of linear equations; Eigen value and eigenvector problems; Ordinary and partial differential equations: Euler, Runge-Kutta and finite difference methods; Solution to initial and boundary value problems; Problems on chemical kinetics; Solution of Newton's equation of motion; Solution of time-dependent Schrodinger equation for simple potentials. Approaches to solve the time-independent Schrodinger's equation, Use of standard available softwares to perform simple quantum chemical calculations.

Text Books:

1. S. J. Chapman, Fortran 90/95 for Scientists and Engineers, 2nd Ed., McGraw-Hill, 2003.
2. S. C. Chapra and P. Canale, Numerical Methods for Engineers 4th Ed., Tata McGraw -Hill, 2002.
3. P. W. Atkins and R. S. Friedman, Molecular Quantum Mechanics, 5th Ed., Oxford University Press, 2010.

References:

1. Numerical Recipes in FORTRAN/C by W. H. Press , S. A. Teukolsky, W. T. Vetterling and B. P. Flannery, Cambridge University Press, 2nd edition, 1996.
2. J. M. Thijssen, Computational Physics, 2nd Ed. Cambridge Uni. , 2007.
3. F. Jensen, Introduction to Computational Chemistry, 3rd edition, Wiley, 2017

CH xyz: Application of nanomaterials (3-0-0-6)

History of nanomaterials; Origin of size-dependent properties; Zero, One, and Two dimensional nanomaterials; Syntheses and Characterization of nanomaterials.

Nanocatalysts; Nanocomposites; Smart materials; Self-healing materials; Magnetic nanomaterials; Hydrogels and Aerogels; Nanosensors;

Nanofluidics; Nanochannel fabrication techniques; Effect of surface charge; Ionic current rectification; Streaming potential; Water Desalination; Reverse electrodialysis; Fuel cells; Water splitting.

Nanotoxicology; Environmental, health and ethical concerns.

Text Books

1. Introduction to Nanotechnology, 1st Edition, Frank J. Owens, Wiley, 2010.
2. A Textbook of Nanoscience and Nanotechnology, T. Pradeep Tata McGraw-Hill Education, 2003
3. C. P. Poole (Jr.) and F. J. Owens, Introduction to Nanotechnology, Wiley Interscience, John Wiley and Sons, Hoboken, New Jersey, 2003.
4. G. A. Ozin and A. C. Arsenault, Nanochemistry: A Chemical Approach to Nanomaterials, RSC Publishing, Royal Society of Chemistry, U.K, 2005.

References

1. Chemistry of Nanomaterials, C.N.R. Rao, A. Muller and A.K. Cheetham, Wiley-VCH, Weinheim, 2004. Reprinted 2006.
2. Nanofluidics: Nanoscience and Nanotechnology, Editors: Joshua Edel, Andrew deMello, RSC Nanoscience & Nanotechnology), 2008
3. Nanofluidics and Microfluidics, 1st Edition, Shaurya Prakash Junghoon Yeom, Elsevier, 2014

4. Nanocrystals: Synthesis, Properties and Applications, C.N.R. Rao, P.J. Thomas, G.U. Kulkarni, Springer-Verlag, 2007, Chinese Edition 2012.

CH 323 Polymer Chemistry (3-0-0-6)

Introductory concepts, definition, common system chemistry and classification of polymers, resins, rubber, plastics; Conformations and properties of various types of polymers; Characterization: molecular weight studies and molecular weight distribution; Mechanistic aspects: addition, ionic, emulsion, suspension, aqueous, coordination, condensation polymerization; Relevant aspects of physical properties of polymer systems, rheological properties; Unit operations: calendering, extrusion and molding; fabrication processes, degradation and stabilization of polymer systems; Polymer Industry: manufacturing of some industrially important polymers (like PVC, Polyethylene, synthetic rubber, and synthetic fiber) and their characterization; Polymer Processing, Polymer additives and Curatives; Recent development in the field of biodegradable polymers.

Texts:

1. G.S. Misra, *Introduction to Polymer Chemistry*, Wiley Eastern, New Delhi, 1993.
2. J. R. Fried, *Polymer Science and Technology*, Prentice Hall, Englewood Cliffs, 1995.

References:

1. R. E. Fornes and R. D. Gilbert, *Polymer and Fiber Science: Recent Advances*, VCH, New York, 1991.
2. L.H. Sperling, *Introduction to Physical Polymer Science*, John Wiley & Sons, New York, 1992.
3. S. R. Sandler and W. Koro, *Polymer Syntheses*, Academic Press, Boston, 1992.

CH 334 Chemical Technology Lab - III (0-0-6-6)

Experiments based on various physical properties such as viscosity, surface tension, optical rotation and refractive index, light absorption and emission (spectroscopy); Experiments based on chemical kinetics and thermodynamics: determination of order of simple reactions, energy

of activation, equilibrium constants, determination of thermodynamic functions; Experiments based on EMF and conductance measurements: determination of electrode potentials, solubility product, pH equivalent conductance; Experiments based on micro-fluidics; Experiments based on surface and interfacial chemistry: surface tension, CMC measurements, HLB values, adsorption isotherms and determination of surface area; Experiments based on phase equilibria: Study of binary and ternary liquid systems; Experiments based on deposition of thin polymer film on substrates and its characterization; Experiments based on syntheses of nano-particles and their characterizations.

Texts/References:

1. B. Viswanathan and P. S. Raghavan, *Practical Physical Chemistry*, Viva Books Private Ltd., 2005.
2. D. P. Shoemaker, C. W. Garland and J. W. Nibler, *Experiments in Physical Chemistry*, 5th Ed., McGraw- Hill International Editions, 1989.
3. J. M. Postma, J. L. Roberts (Jr.) and J. L. Hollenberg, *Chemistry in the Laboratory*, 6th Ed., W. H. Freeman and Company, 2004.
4. V. D. Athawale and Parul Mathur, *Experimental Physical Chemistry*, New Age International Publishers, 2001.
5. R. A. Day (Jr.) and A. L. Underwood, *Quantitative Analysis*, 6th Ed., Prentice-Hall of India Pvt. Ltd., 2006.
6. G. D. Christian, *Analytical Chemistry*, 6th Edition, John Wiley & Sons, Inc. ,2003.

CH 401 Modern Chemical Technology (3-0-0-6)

Fine chemicals and their synthesis: bio-catalysis, enantio-selective catalysis; catalysis in fine chemicals: mechanism of catalysis, homogeneous and heterogeneous catalysis; catalyst performance, phase transfer catalysis; Selectivity engineering, Process development, Energy and its biological resources; Bio-Fuels: Biofuel feedstocks: sugar, starch, lignocelluolosic, plant and animal fats feedstock; Market and product process of bioethanol; Raw materials to produce low cost bio-diesel; Harvesting energy from biochemical resources.

Texts:

1. A. Cybulski, J. A. Moulijn, M. M. Sharma, and R. A. Sheldon, *Fine Chemicals Manufacturing and Engineering* , Elsevier Science, 2001.
2. C. M. Drapcho, N. P. Nhuan and T. H. Walker, *Biofuels Engineering and Process Technology*, McGraw Hill, 2008.

References:

1. P. Pollak, *Fine Chemicals: The industry and the Business*, John Wiley and Sons, 2007.
2. A. Nag, *Biofuels refining and performance*, McGraw Hill, 2008.
3. D. M. Mousdale, *Biofuels: Biotechnology, Chemistry and Sustainable Development* CRC Press, 2008
4. R. N. Shreve and J. A. Brink, *Chemical Process Industries*, 4th Ed., International Students Edition,1977.
5. G. F. Austin, *Shreve's Chemical Process Industries*, 5th Ed., McGraw Hill Pub., 1984.

Department Electives

CH 431: Quantum Molecular Dynamics (3-0-0-6)

The time-dependent Schrödinger's equation, Wavepackets, Correspondence between classical and quantum dynamics, The Wigner representation and the density operator, Correlation functions, Approximate solutions of the time-dependent Schrödinger's equation, Methods of quantum propagation of wave functions: Split operator method and the fast Fourier transform, The Born-Oppenheimer approximation and potential energy surfaces, Electronic absorption and Emission spectroscopy, Two-level system, Effect of strong fields, Variational formulation of control of chemical reactions, photodissociation, Reactive scattering problems.

Text Book

1. Introduction to quantum mechanics: A time-dependent perspective, D. J Tannor, 2007, Universty Science Books.

Reference

1. S. A. Rice, and M. Zhao, Optical Control of Molecular Dynamics 1st Edition, Wiley-Interscience, 2000

CH 427 Medicinal Chemistry (3-0-0-6)

Introduction to medicinal and pharmaceutical chemistry: Methods of classification of drugs based on structure and biological activity; Study of the chemistry and synthesis of the following classes of drugs: Anti-infective agents such as antiseptic and disinfectant, antibiotics (including stability and degradation products), antiparasitic, antiamoebic, antihelminitic, antimycobacterial, antifungal, anticancer, antiviral; Non-steroidal anti-inflammatory agents (NSAIDs); Drugs used in hypertensive, vasodilator, immunopharma-cology; Large scale synthesis: bench-scale experimentation, scale up, scale up from bench to pilot plant, commercial scale operation, example - Nevirapine.

Texts:

1. D. A. Williams and T. L. Lemke, *Foye's Principles of Medicinal Chemistry*, Lippincott Williams & Wilkins, Philadelphia, 2002.
2. D. Lednicer, *Strategies for Organic Drug Synthesis and Design*, John Wiley & Sons Inc., New York, 1998.

References:

1. D. J. Abraham (ed.), *Burger's Medicinal Chemistry and Drug Discovery, Vol. 1 - 6*, Wiley-Interscience, 2003.
2. D. Lednicer, *Organic Chemistry of Drug Synthesis, Vol. 1 - 6*, John Wiley & Sons Inc., New York, 1977.
3. S. Warren, *Organic Synthesis: The Disconnection Approach*, John Wiley & Sons, 2002.

CH 428 Drug Design and Development (3-0-0-6)

Drug targets; Pharmacokinetics: ADME, administration and dosing; Drug testing: *in vivo*, *in vitro*; Drug discovery: natural lead, synthetic lead, combinatorial synthesis; Pharmacokinetics based drug design; Computer aided drug design: Principles of QSAR, 2D QSAR, 3D QSAR; Chemical development, Patenting, Process development; Toxicology, Pharmacology, Drug metabolism, Clinical trials, Commercialization: regulatory affairs, pipeline development, pharmaceutical market places, business opportunities.

Texts:

1. G. Thomas, *Fundamentals of Medicinal Chemistry,* John Wiley & Sons Ltd., 2006.
2. G. Patrick, *Instant Notes: Medicinal Chemistry,* Viva Books Pvt. Ltd., 2002.

References:

1. G. Patrick, *An Introduction to Medicinal Chemistry,* Oxford University Press, 2001.
2. T. Nogrady, *Medicinal Chemistry: A Biochemical Approach,* Oxford University Press, 2004.
3. S. Pidgeon, *Wiley handbook of Current and Emerging Drug Therapies*, *Vol. 4,* Wiley-Interscience, 2007.

CH 417 Organometallic Chemistry (3-0-0-6)

18-electron rule; Stabilisation of low oxidation state of metals; Metal carbonyls, nitrosyls, cabonyl hydrides, isolobal analogy, dioxygen and dinitrogencompoun ds; Metal alkyls, carbenes, carbynes, alkenes, alkynes, and allyl complexes; Hydrides, Metallocenes, Metal arene complexes; Carbonylate anions, agostic interaction, Oxidative addition and reductive elimination, insertion and elimination reactions; Industrial organometallic catalysis: Homogeneous and heterogeneous catalysis; Organomeatllic reagents in drugs synthesis Fluxional molecules; Metal-Metal bonding and Metal clusters; Organometallic materials : synthesis and applications; Biological and environmental aspects of organometallic compounds.

Texts:

1. J. E. Huheey, E. A. Keiter and R. L. Keiter, *Inorganic Chemistry: Principles of Structure and Reactivity;* 4th Ed., Harper Collins, 1993.
2. B. E. Douglas, D. H. McDaniel and J. J. Alexander, *Concepts and Models of Inorganic Chemistry*; 3rd Ed., John Wiley, 1993.

References:

1.C. Elschenbroich and A. Salzer, *Organometallics*; 2nd Ed., VCH, 1995.

2. A. Yamamoto, *Organotransition Metal Chemistry: Fundamental Concepts and Applications*; John Wiley, 1986.

3. R. H. Crabtree, *Organometallic Chemistry of the Transition Metals*; 2nd Ed., John Wiley, 1993.

4. F. A. Cotton and G. W. Wilkinson, *Advanced Inorganic Chemistry*; 5th Ed., John-Wiley & Sons, 1988.

CH 418 Biological Chemistry of Metal Ions (3-0-0-6)

Essential and trace metals; Role of alkali and alkaline earth metal ions, Na^+-K^+ Pump, ionophores and crown ethers; Metal ion transport and storage: Ferritin, Transferrin, Siderophores and metallothionein; Electron Transfer: Cytochromes, Fe-S proteins and Copper proteins; Oxygen transport and storage: Hemoglobin, myoglobin, hemerythrin, hemocyanin; Oxygen activation: Cytochrome P450, Cytochrome c oxidase; Others: Catalase, peroxidase, superoxide dismutase, alcohol dehydrogenase, carbonic anhydrase, carboxypeptidase, xanthine oxidase, nitrogenase, vitamin B12 coenzyme, photosystem I and II, oxygen evolving center; Hazardous coordination complexes; Coordination complexes as medicines.

Texts:

1. S. J. Lippard and J. M. Berg, *Principle of Bioinorganic Chemistry*, University Science Books, 1994.

2. J. J. R. F. da Silva and R. J. P. Williams, *The biological chemistry of the elements: the inorganic chemistry of life;* 2nd Ed., Oxford University Press, New Delhi, 2006.

References:

1. J. E. Huheey, E. A. Keiter and R. L. Keiter, *Inorganic Chemistry: Principles of Structure and Reactivity;* 4th Ed., Harper Collins, 1993.

2. D. F. Shriver and P. W. Atkins, *Inorganic Chemistry*; 3rd Ed., Oxford University Press, New Delhi, 2004.

CH 419 Consumer Chemistry (3-0-0-6)

Chemistry in the laundry: Soaps, domestic laundry detergents, other household cleaning agents, chemistry of washings.

Chemistry in the kitchen: Butter, margarine and other fats, oils and waxes, body fat, fish oils, chocolate, cholesterol, prostaglandins, antioxidants, chemistry of cooking.

Chemistry in the boudoir: Chemistry of cosmetics, lipsticks, toothpaste, deodorants, sunglasses, baby care products.

Chemistry in the garden: Pesitcides and alternatives, fertilizers, insect repellents, swimming pool chemistry.

Chemistry in the medicine cabinet: Medicinal chemistry of drugs, drugs action, tranquillisers, anaesthetic drugs.

Chemistry in the dining room: Food additives, alchoholic products, caffeine, nutrition, digestion, allegies.

Text Book:

Consumer Chemistry, Sarah Bent Ransom, John Chiocca and Robert Van Reen, 2005

CH 426 Green Chemistry and Technology (3-0-0-6)

Principles and Concepts of Green Chemistry: Sustainable development, atom economy, reducing toxicity; Waste: production, problems and prevention, sources of waste, cost of waste, waste minimization technique, waste treatment and recycling; Alternate solvents: safer solvents, green solvents, water as solvents, solvent free conditions, ionic liquids, super critical solvents, fluorous biphase solvents; Alternative Energy Source: Energy efficient design, photochemical reactions, microwave assisted reactions, sonochemistry and electrochemistry; Process and Operations: Industrial preparation, reaction, reactor design, inherently safer design (ISD), process intensification (PI), in process monitoring, micromixers, unit operations; Reaction with separation operations, process integration; Industrial Case Studies: Greening of acetic acid manufacture, EPDM rubbers, Vitamin C, Leather manufacture (tanning, fatliquoring), green dyeing, polyethylene, ecofriendly pesticides, sugar and distillery industry, paper and pulp industry, pharmaceutical industry; An integrated approach to green chemical industry.

Texts:

1. M. Lancaster, *Green Chemistry: An Introductory Text*, Royal Society of Chemistry, 2002.

2.M. Doble and A. K. Kruthiventi, *Green Chemistry and Engineering*, Academic Press, Amsterdam, 2007.

References:

1. P. T. Anastas and J.C. Warner, *Green Chemistry, Theory and Practice*, Oxford, 2000.

2. V. K. Ahluwalia, *Green Chemistry: Environmentally Benign Reactions*, Ane Books India, New Delhi, 2006.

3. M. M. Srivastava and R. Sanghi, *Chemistry for Green Environment*, Narosa, New Delhi, 2005.

4. R.E. Sanders, *Chemical Process Safety: Learning from Case Histories*, Butterworth Heinemann, Boston, 1999.

5. P. Tundo, A. Perosa, and F. Zecchini (eds.), *Methods and Reagents for Green Chemistry*: *An Introduction*, Wiley, 2007.

Open Electives

CH 429 Petroleum and Petrochemicals (3-0-0-6)

Origin, formation and composition of petroleum, petroleum processing: fractionation, blending of gasoline, gasoline treatment, kerosene treatment, treatment of lubes, petroleum wax and purification; Thermal and catalytic processes: thermal cracking, catalytic cracking, catalytic reforming, naphtha cracking, coking, hydrogen processes, alkylation, isomerization processes; polymer gasoline, asphalt, upgradation of heavy crudes; Specialty products: industrial gases, liquid paraffin, petroleum jelly; Sources of petrochemicals; Synthesis of methanol, formaldehyde, acetylene, synthetic gas, ethanol, ethylene, ethylene glycol, vinyl acetate, acrylic acid and acrylates, acrylonitrile, acetone, acetic acid, chloroprene, vinyl chloride, vinyl acetate, acrylonitrile, propylene, butadiene, butanes, isobutene, adipic acid, adiponitrile, benzene, toluene, xylene, phenol, styrene, phthalic acid, phthalic anhydride and their applications in chemical industry.

Texts:

1. B. K. B. Rao, *Modern Petroleum Refining Processes*, 4th Ed., Oxford & IBH Publishing Co. Pvt Ltd., New Delhi, 2002.
2. P. Wiseman, *Petrochemicals*, John Wiley & Sons, 1986.

References:

1. R. A. Meyers, *Handbook of Petroleum Refining Processes*, 3rd Ed., McGraw-Hill, 2004.
2. S. Raseev, *Thermal and Catalytic Processes in Petroleum Refining*, Marcel Dekker, Inc., 2003.

CH 437 Chemical Approaches to Nanoscale Science and Technology (3-0-0-6)

Properties of materials with nanoscale dimensions; Zero, one, two and threedimensional materials; Inorganic Nanomaterials: Metallic nanocrystals with special emphasis on coinage metals, semiconductor nanocrystals, quantum dots, magnetic materials, syntheses, characterizations and properties; Carbonnantubes; Organic and biological nanostructures; Measurements: Optical spectroscopy and microscopy, scanning probe microscopy, scanning electron microscopy, transmission electron microscopy and X-ray diffraction; Applications: Catalysts, sensors, actuators, display systems, molecular devices and nanobiotechology.

Texts:

1. C. P. Poole (Jr.) and F. J. Owens, *Introduction to Nanotechnology*, Wiley Interscience, John Wiley and Sons, Hoboken, New Jersey, 2003.
2. G. A. Ozin and A. C. Arsenault, *Nanochemistry: A Chemical Approach to Nanomaterials*, RSC Publishing, Royal Society of Chemistry, U.K, 2005.

References:

1. L. M. Liz-Marsan and P. V. Kamat, *Nanoscale Materials*, Kluwer Academic Publishers, Boston, USA, 2003.
2. D. A. Bonnel, Scanning *Probe Microscopy and Spectroscopy: Theory, Techniques and Application*s. 2nd Ed.. New York, Wiley-VCH, 2001.
3. S. Amelinckx, *Electron Microscopy: Principles and Fundamentals*, Weinheim, VCH, 1997.
4. B. Valeur, *Molecular Fluorescence: Principles and Applications*, Wiley-VCH Verlag, GmbH, Weinheim (Federal Republic of Germany), 2002.

5. D. Astruc, *Nanoparticles and Catalysis*, Wiley-VCH, Wiley-VCH Verlag GmbH and Co. KGaA, Weinheim, 2008.

CH 438 Application of Statistical Mechanics to Chemistry (3-0-0-6)

Introduction and reviews of classical mechanics, quantum mechanics and thermodynamics; Microstates, macrostates, canonical, grand canonical and microcanonical ensemble; Boltzmann distribution for distinguishable particles; The emergence of temperature from conditions for equilibrium; postulate for entropy; Partition function for a single particle; Thermodynamic potentials and variables in terms of partition function, energy degeneracy and partition functions, many (weakly interacting) particle partition function, derivation of thermodynamics of a simple harmonic oscillator, distinguishable and indistinguishable particles, counting states of a gas of indistinguishable particles, density of states, partition function of an ideal gas, derivation of the equation state of an ideal gas;the Gibbs paradox and indistinguishibility;Application of the theory of statistical mechanics to the chemical problems related to rotational specific heat of gases; Maxwell-Boltzmann distribution of velocities; Quantum statistics (Bose-Einstein and Femi-Dirac) for indistinguishable particles; Photon gas; Density of states for photons; Black body radiation; Debye frequency and specific heat of phonons, heat capacity of a Fermi gas, the classical limit from the quantum mechanical expression for paritition function, distribution functions in classical monatomic liquids, direct correlation function, density expansions of the various distribution functions.

Texts:

1. D. A. McQuarrie, *Statistical Mechanics*, University Science Books, 2000.
2. R. K. Pathria, *Statistical Mechanics*, Butterworth-Heinemann, 1996.

Reference:

1. K. Huang, *Statistical Mechanics*, John Wiley Asia, 2000.