B. Tech in Chemical Science and Technology

Course Structure

Semester - 1

Course No	Course Name	L-T-P-C
MA-101	Mathematics - I	3-1-0-8
CH-101	Chemistry	3-1-0-8
CH-110	Chemistry Laboratory	0-0-3-3
PH-101	Physics-1	2-1-0-6
ME-111	Engineering Drawing	2-0-3-7
ME-110	Workshop - I	0-0-3-3
EC-101	Electrical Sciences	3-1-0-8
HS-1xx	English*/HSS Elective	3-0-0-6
SA 101#	Physical Training I	PP/NP
	NCC / NSS / NSO	0-0-0-0
	Total Credits:	16-4-9-49

Semester - 2

Course No	Course Name	L-T-P-C
MA-102	Mathematics - II	3-1-0-8
ME-101	Engineering Mechanics	3-1-0-8
CS-101	Introduction to Computing	3-0-0-6
PH-102	Physics - II	2-1-0-6
BT-101	Modern Biology	3-1-0-8
EC-102	Basic Electronics Laboratory	0-0-4-4
CS-110	Computing Laboratory	0-0-3-3
PH-110	Physics Laboratory	0-0-3-3
SA 102#	Physical Training II	PP/NP
	NCC / NSS / NSO	0-0-0-0
	Total Credits:	14-4-10-46

Semester - 3

Course No	Course Name	L-T-P-C
CS-201	OOP and Data Structures	3-0-3-9
MA 201	Mathematics III	3-1-0-8
HS 2xx	HSS Elective	3-0-0-6
CH 211	Preliminaries of Inorganic Chemistry	3-1-0-8
CL 202	Fluid Mechanics	3-1-0-8
CH 221	Principles of Organic Chemistry	3-0-0-6
SA 201#	Physical Training III	PP/NP
	NCC / NSS / NSO	0-0-0-0
	Total Credits:	18-3-3-45

Semester 4

Course No	Course Name	L-T-P-C
HS-2xx	HSS Elective	3-0-0-6
XX 2xx	Science Elective	3-0-0-6
CH 212	Chemistry of Non Metals	3-1-0-8
CH 222	Mechanism of Organic Reactions	3-1-0-8
CH 223	Chemical Technology Lab I	0-0-9-9
CH 332	Introduction to Quantum Chemistry	3-1-0-8
SA 202#	Physical Training IV	PP/NP
	NCC / NSS / NSO	0-0-0-0
	Total Credits:	15-3-9-45

Semester - 5

Course No	Course Name	L-T-P-C
CH 231	Introduction to Chemical Thermodynamics and Equilibrium	3-1-0-8
CH 313	Chemistry of Metals	3-1-0-8
CH 314	Chemical Technology Lab II	0-0-9-9
CH 324	Applied Organic Chemistry	3-1-0-8
PH 415	Solid State Physics	3-1-0-8
CH 431	Group Theory and Spectroscopy	3-1-0-8
	Total Credits:	15-5-9-49

Semester - 6

Course No	Course Name	L-T-P-C
PH 308	Numerical Methods and Computational Physics	2-0-2-6
HS 3xx	HSS Elective	3-0-0-6
CH 301	Spectroscopic Techniques in Chemistry	3-1-0-8
CH 333	Computational Chemistry	2-0-3-7
CH 334	Chemical Technology Lab III	0-0-9-9
CH 335	Chemical Kinetics and Electrochemistry	3-1-0-8
	Total Credits:	14-3-11-44

Semester - 7

Course No	Course Name	L-T-P-C
CH 401	Modern Chemical Technology	3-1-0-8
CH 402	Technical Report and Presentation	0-0-3-3
CH 498	Project I	0-0-8-8
XX 4xx	Open Elective I	3-0-0-6
CH 4xx	Elective I	3-0-0-6
CH 4xx	Elective II	3-0-0-6
	Total Credits:	12-1-11-37

Semester - 8

Course No	Course Name	L-T-P-C
HS 4xx	HSS Elective	3-0-0-6
XX 4xx	Open Elective II	3-0-0-6
CH 4xx	Elective III	3-0-0-6
CH 499	Project II	0-0-16-16
	Total Credits:	9-0-16-34

Elective Courses

CH 403 Environmental Chemistry
CH 404 Introduction to Polymer Chemistry
CH 414 Industrial Chemistry
CH 426 Green Chemistry and Technology
CH 427 Medicinal Chemistry
CH 428 Drug Design and Development
CH 429 Petroleum and petrochemicals
CH 437 Chemical Approaches to Nanoscale Science and Technology
CH 438 Application of Statistical Mechanics to Chemistry

CH 211: Preliminaries of Inorganic Chemistry (3–1–0–8)

Acids and bases: classification, Arrhenius, Bronsted-Lowry, Lux-Flood, 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, analysis of redox cycle, Frost, Latimer and Pourbaix diagram; redox principles involved in the extraction of the elements; chemical bonding: valence bond theory, hybridization, VSEPR theory, molecular orbital theory, homonuclear and heteronuclear diatomic molecules, bond energy, bond order, percentage ionic character, polarizing power, Fajan's rule, hydrogen bond, van der Waals forces; coordination compounds: Werner's coordination theory and its experimental verification, effective atomic number concept, nomenclature of coordination compounds, isomerism, chelate effect, macrocyclic ligands; bonding in coordination complexes: valence bond theory, crystal-field theory, d-orbital splitting in octahedral, tetrahedral, square planar geometries; non-aqueous solvents: types of solvents, general characteristics, reactions in non-aqueous solvents with reference to liquid NH_3 and liquid SO_2, ionic liquids.

Text Books:

1. D. J. Shriver, P. W. Atkins, C. H. Langford, *Inorganic Chemistry*, 2nd Ed, Oxford (1994).

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

3. J. E. Huheey, E. A. Keiter and R. L. Keiter, *Inorganic Chemistry: Principles of Structure and Reactivity*, Dorling Kindersley (2006).

CH 212: Chemistry of Non Metals (3–1–0–8)

Non metals: relative position in the periodic table, characteristics, brief description of their periodic properties; chemistry of hydrogen: properties and formation of hydrogen, hydrides; chemistry of boron: metal borides, boron Halides, oxygen compounds of boron, hydrides of boron, nitrogen compounds of boron; chemistry of carbon and silicon: allotrope, oxides and oxyacids, silicates, silicones; chemistry of nitrogen and phosphorous: chemistry of nitrogen, nitrogen oxides and nitrogen hydrides, 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 oxygen and sulfur: chemistry of oxygen, oxides, peroxides, superoxides, ozone, chemistry of sulfur and sulfur oxides, differences between the chemistry of sulfur and oxygen; chemistry of the halogens: pseudo-halogen, interhalogen, oxides and oxyacids, polyhalides; chemistry of the rare gases: chemistry of xenon, structure and bonding of xenon compounds.

Text Books:

1. D. J. Shriver, P. W. Atkins, C. H. Langford, *Inorganic Chemistry*, 2nd Ed, Oxford (1994).

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

3. J. E. Huheey, E. A. Keiter and R. L. Keiter, *Inorganic Chemistry: Principles of Structure and Reactivity*, Dorling Kindersley (2006).

CH 221: Principles of Organic Chemistry (3-0-0-6)

Structure and bonding: hybridization, bond theory, van der Waals interactions, charge transfer complexes, hyperconjugation, inductive, resonance and fields effects; bonding and structures of reactive intermediates; cabocation, carbanion, radicals and carbene; conformation and stereochemistry: conformational analysis of cyclohexane and larger ring system, stereogenicity and stereoisomerism, symmetry and stereochemistry, topocity relationship, reaction stereochemistry, stereoselectivity and stereospecificity, stereochemical issues in biology; structure and reactivity: different types of reactions and mechanism, thermodynamic and kinetic requirements, the Hammond postulate, reactivity vs. selectivity, the Curtin-Hammett principle, kinetic vs thermodynamic control, transition states and intermediates, methods of determining mechanism, isotope effects, generation, structure, stability and reactivity of carbocation, carbanion, free radical, carbene and nitrene, substituents effects: fields effects, inductive effects, resonance effects, polarizability effects, steric and solvation effects; Hammett equation and linear free energy relationship, Taft equation; aromatic compounds: sources, nomenclature, structure, aromaticity and antiaromaticity, Huckel's rule, aromatic electrophilic substitution, activating and deactivating substituents.

Text Books:

1. Eric V. Anslyn and Dennis A. Dougherty, *Modern Physical Organic Chemistry*, 1st Ed University Science Books, California (2006).

2. R. T. Morrison and R. N. Boyd, *Organic Chemistry*, 6th Ed, Prantice-Hall (2004).

3. M. B. Smith and J. March, *Advanced Organic Chemistry*, 6th Ed, John Wiley and Sons, Inc (2007).

4. P. Sykes, *A guide to mechanism in Organic Chemistry*, 6th Ed, Pearson Education (2004).

5. I. L. Finar, *Organic Chemistry*, Vol. 1 & 2, 5th Ed, Pearson Education (2005).

CH 222: Mechanism of Organic Reactions (3–1–0–8)

Types of organic reactions, energy considerations, reactive intermediates–carbocations: classical and nonclassical, carbanions, free radicals, carbenes, arynes and nitrenes (with example); methods of determining organic reaction mechanism; product analysis, intermediates, isotope effects, kinetic and stereochemical studies, aliphatic nucleophilic substitution reactions: S_N2 , S_N1 and borderline mechanism, neighbouring group participation, nucleophilicity and solvent effects, leaving group effects, steric and strain effects, effects of conjugates, stereochemistry of nucleophilic substitution; arenium ion mechanism, orientation and reactivity; aromatic nucleophilic substitution reaction , S_NAr, S_N1 benzyne and SRN^1 reaction, free radical reactions: free radical substitution reaction for aliphatic and aromatic substrates; addition reactions: addition to C-C multiple bonds; addition of electrophile, nucleophiles and free radicals, regio and chemoselectivity, orientation and reactivity; addition to carbon-hetero multiple bonds: mechanism of metal hydride reduction of carbonyl compounds, and nitriles, addition of organometallics to carbonyl compounds; elimination reactions: E^2, E^1 and E1cB mechanisms; reactivity: effects of substrate, attacking base, leaving group and medium.

Text Books:

1. J. March, *Advanced Organic Chemistry*, 6th Ed, John Wiely & Sons (2007).

2. J. Clayden, N. Breevers, S. Warren, P. Wothers, *Organic Chemistry*, Oxford University Press (2001).

References:

1. J. M. Hornbook, *Organic Chemistry*, Books Coley (1998).

2. P. Y. Bruice, *Organic Chemistry*, Prentice Hall (1998).

3. P. S. Kalsi, *Organic Reaction and their mechanism*, New Age (1996).

CH 223: Chemical Technology Lab - I (0-0-9-9)

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.

Text Books:

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, A.R. Tatchell, *Vogel's textbooks of practical organic chemistry*, 5th Ed, ELBS Longman (1994).

CH 231: Introduction to Chemical Thermodynamics and Equilibrium (3-1-0-8)

Ideal gases, real gases, critical state; thermodynamic laws; reversible and irreversible processes; Thermochemistry: Hess's law, Kirchoff's equation; entropy; application of thermodynamic laws; Carnot cycle; Clausius inequality; equations of state; Gibbs and Helmholtz free energies; Maxwell equations and thermodynamic properties of pure substances; Colligative properties; chemical potential; chemical equilibria; equilibrium constant; Le Chatelier principle; Clapeyron equation; phase equilibria: Gibbs phase rule, one component systems and two component systems – simple eutectic, Solid solutions – congruent melting and incongruent melting.

Text Books:

1. G. W. Castellan, *Physical Chemistry*, 3rd edition, Addison Wesley Publishing Company (1983).
2. P. W. Atkins, J. de Paula Atkins ' *Physical Chemistry*, 7th Ed, Oxford University Press (2002).

CH 301: Spectroscopic Techniques in Chemistry (3–1–0–8)

Vibrational spectroscopy: Symmetry and shapes of ABn systems, modes of bonding in ambidentate ligands. Characteristic vibrational frequencies of different functional groups, effect of hydrogen bonding and solvent effect on vibrational frequencies, overtones, combination and Fermi resonance bands. UV-Vis: Electronic spectra of transition metal complexes, Woodward rule for organic compounds. Nuclear Magnetic Resonance: Basic NMR spectroscopy, resonance, chemical shift, spin-spin interaction, shielding mechanism, complex spin-spin interaction, virtual coupling stereochemistry, nuclear magnetic double resonance, nuclear overhauser effect (NOE), resonance of other nuclei. ^{13}C NMR: Chemical shift, ^{13}C coupling constants, two-dimensional NMR spectroscopy, NOISY, DEPT, INEPT terminology. Electron Spin Resonance: Hyperfine coupling, spin polarization for atoms and transition metal ions, spin-orbit coupling and significance of g-tensor, application of EPR in radical and transition metal complexes. M□sbauer: Basic principles, spectral parameters and spectrum display, application to the studies of Fe and Sn compounds. Mass: Instrumentation, Mass spectral fragmentation of organic compounds, McLafferty rearrangement.

Text Books:

1. R. M. Silverstein, *Spectrometric Identifications of Organic Compounds,* John Wiley (1991).
2. D.L. Pavia, G. M. Lampman, G. S. Kriz, *Introduction to Spectroscopy*, Harcourt College Publisher, NY (2001).

References:

1. William Kemp, *Organic Spectroscopy*, 3rd Ed, ELBS (1994).
2. A. B. P. Lever, *Inorganic Electronic Spectroscopy*, 2nd Ed, Elsevier (1984).
3. R. S. Drago, *Physical Methods in Chemistry*, Saunders (1992).

CH 313: Chemistry of Metals (3-1-0-8)

Classification and general properties, occurrence, isolation, oxidation states, chemical and redox reactions of the metals. Alkyls, halides, hydrides, oxides, alkoxides and other coordination and organometallic compounds of the metals. Metallic chains, sheets and clusters. Metal silicates, zeolites and polyoxo-metallates. Metals and alloys, ceramic materials, intermetallic compounds and zintl phases. Applications of metals and their derivative systems in industry. Materials science and technology: optoelectronic properties, magnetism, electrical conductivity and surface coating technology.

Text Books:

1. N. N. Greenwood and A. Earnshaw, *Chemistry of the Elements,* 2nd Ed, London: Butterworth Heinmann (1997).
2. J. McMurry and R. C. Fay, *Chemistry*, 5th Ed, Delhi: Pearson Education (2008).
3. D. Thompson, *Insights into Specialty Inorganic Chemicals*, The Royal Society of Chemistry , Cambridge (1995)

References:

1. G. Wolfsberg, *Inorganic Chemistry*, 1st Indian Ed, University Science Books (2002).
2. P. K. Dutt, *Concepts of Chemistry*, Levant Book (2004)
3. D. W. Bruce and D. O'Hare, *Inorganic Materials*, 2nd Ed., John Wiley & Sons (1999)
4. T. T. Kodas and M. J. Hampden-Smith, *The chemistry of Metal CVD,* Wiley-VCH (1994).

CH 314: Chemical Technology Lab II (0-0-9-9)

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.

Text Books:

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).

Reference:
1. K. Hutchings, *Classic Chemistry Experiments*, The Royal Society of Chemistry, London (2000

CH 324: Applied Organic Chemistry (3-1-0-8)

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 behaviour, molecular structure and liquid crystals, application of liquid crystal.

Text Books:

1. R. T. Morrison and R. N. Boyd, *Organic Chemistry,* 6th Ed*,* Prentic – Hall (2004).
2. R. V. Gadag and A. N. Shetty, *Engineering Chemistry*, I. K. International (2006).
3. Billmeyer, *Text book of Polymer Science,* 3rd Ed, John Wiley & Sons (1984).
4. Malcolm P. Stevens, *Polymer Chemistry,* 3rd Ed, Oxford University Press Inc. (1998).

Reference:

1. I. L. Finar, Organic Chemistry, Vol. 1 & 2, 5th Ed, Pearson education (2005).
2. D. Singh, B. Deshwal and S. K. Vats, *Comprehensive Engineering Chemistry,* I. K. International, Mumbai (2007).

CH 332: Introduction to Quantum Chemistry (3-1-0-8)

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 viz., 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 variational methods 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.

Text Books:

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

References:

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

CH 333: Computational Chemistry (2-0-3-7)

Computer programming in FORTRAN; Molecular modeling – Determination of properties of molecules, charge distribution, viewing the orbitals and vibrational spectra; Biophysical properties of membrane bilayer containing phospholipid and cholesterol; Molecular dynamics: Conformation of protein; Quantum wave packet dynamics: Calculation of auto-correlation function, Fourier analysis, Laser matter interaction using two level problem; Kinetics: Simulation of Ozone kinetics, loss mechanism due to chloro-fluro carbon, day night cycle; Spectra

Text Books:

1. M. Metcalf, and J. Reid, Fortran 90/95 explained, 2nd Edition, Oxford University Press, (1999).
2. Handouts will be given for each experiment.
3. Web resources. of I2: Calculation low and high resolution spectra, Morse potential and their eigenvalue and eigenfunction, Frank-Condon Factors.

CH 334: Chemical Technology Lab III (0-0-9-9)

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 microfluidics. 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 nanoparticles and their characterizations.

References:

1. B. Viswanathan and P. S. Raghavan*, Practical Physical Chemistry*, Viva Books Private Limited (2005).
2. David P. Shoemaker, Carl W. Garland and Joseph W. Nibler, *Experiments in Physical Chemistry,*5th Edition, *McGraw-Hill International Editions* (1989).

3. James M. Postma, Julian L. Roberts, Jr., J. Leland Hollenberg, *Chemistry in the Laboratory*, 6th Edition, 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 Edition, Prentice-Hall of India Private Limited (2006).
6. Gary D. Christian, *Analytical Chemistry*, 6th Edition, John Wiley & Sons, Inc. (2003).
7. Frank Settle, *Handbook of Instrumental Techniques for Analytical Chemistry*, Pearson Education Pvt. Limited (2004).

CH 335: Chemical Kinetics and Electrochemistry (3–1–0–8)

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.

Text Books:

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

CH 401: Modern Chemical Technology (3–1–0–8)

Fine chemicals and their synthesis: biocatalysis, enantioselective 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, BioFuels: 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.

Text Books:

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, 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. David M. Mousdale. *Biofuels: Biotechnology, Chemistry and Sustainable Development* CRC Press 2008
4. R. N. Shreve, J. A. Brink, *Chemical Process Industries*, 4th Ed. (International students Ed.).
5. G. F. Austin, *Shreve's Chemical Process Industries*, 5th Ed., McGraw Hill Pub.

CH 402: 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*, Prentice Hall, 2nd Ed. 1994.

CH 403: 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 Chemsitry : A Practical Guide for Environmental Professionals*, CRC Press.2000.

CH 404: Introduction to 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 414: Industrial Chemistry (3-0-0-6)

Hydrazine: Manufacturing of Hydrazine, Raschig Process, Urea Process, Bayer Process, H2O2 Process, Use of hydrazine viz. 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, Metallic hard materials and Fibers: 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 TiO2 Pigments, Applications for TiO2 Pigments, Lithopone and Zinc Sulfide Pigments, Iron Oxide pigments, Chromium(III) Oxide Pigments, Magnetic Pigments, Manufacture of Magnetic Pigments.

Texts/References:

1. A. Heaton, *An introduction to Industrial Chemistry*, 3rd Ed, Blackie Academic, 1996.
2. T.W. Swaddle, *Inorganic Chemistry: An Industrial and Environmental Perspective*, Academic Press, San Diego, 1997.
3. K. Weissermel and H.J. Arpe, *Industrial Organic Chemistry*, 2nd Ed, Weinheim, VCH, 1996.
4. K. H. Davis and F. S. Berner, *Handbook of Industrial Chemistry*, Vols. 1 and 2, CBS, New Delhi, 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, Lather 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, 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, F. Zecchini (Ed.), *Methods and Reagents for Green Chemistry*: *An Introduction*, Wiley, 2007.

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: 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 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/References:

1) B. K. B. Rao, *Modern Petroleum Refining Processes*, 4th Ed., Oxford & IBH Publishing Co. Pvt Ltd., New Delhi, 2002.
2) R. A. Meyers, *Handbook of Petroleum Refining Processes* , 3rd Edition, McGraw-Hill, 2004.
3) P. Wiseman, *Petrochemicals*, John Wiley & Sons, 1986.
4) S. Raseev, *Thermal and Catalytic Processes in Petroleum Refining*, Marcel Dekker, Inc., 2003.

CH-431: Group Theory and Spectroscopy (3–1–0–8)

Group Theory: Definition of group, symmetry, point groups, representation of group, orthogonality theorem, irreducible representation, character table, direct sum, direct product, derivation of projection operator. Spectroscopy: Electromagnetic radiation and its interaction with matter. Uncertainty principle: Natural line width and broadening. Microwave: classification of molecules, rigid rotor model, selection rules, intensity of spectral lines, effect of isotopic substitution. Stark effect. Infrared: Review of harmonic oscillator, selection rules, vibrational energy of diatomic molecules, zero point energy, force constant and bond strength; anharmonicity, Morse potential energy diagram, vibration-rotation spectroscopy, P, Q, R, branches. Breakdown of Born-Oppenheimer approximation, vibration of polyatomic molecules. normal mode of vibration, group frequencies, overtone, hot bands. Raman: Classical and quantum theories of Raman effect, pure rotational, vibrational and vibrational-rotational Raman spectra, selection rules, mutual exclusion principle. Resonance Raman. Molecular Spectroscopy: Energy levels, MO, vibronic transitions, Franck-Condon principle, electronic spectra of polyatomic molecules. Emission spectra, radiative and non-radiative decay, internal conversion. Photoelectron spectroscopy.

Text Books:

1. Chemical Applications of Group Theory by F.A. Cotton, Wiley Interscience, 1990, 3rd Ed.
2. Fundamentals of Molecular Spectroscopy by C. N. Banwell and E. M. McCash, Tata McGraw Hill, 1994.

References:

1. Group Theory and Quantum Mechanics by M. Tinkham, McGraw Hill, 1964.
2. Introduction to Molecular Spectroscopy by G. M. Barrow, McGraw Hill.
3. Introduction to Atomic Spectra by H. E. White, McGraw Hill, 1934.
4. Modern Molecular Photochemistry by Nicholas J. Turro, University Science Books, 1991.

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

Properties of materials with nanoscale dimensions. Zero, one, two and three–dimensional materials. Inorganic Nanomaterials: Metallic nanocrystals with special emphasis on coinage metals, semiconductor nanocrystals, quantum dots, magnetic materials. Syntheses, characterizations and properties. Carbon nantubes. 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 andApplication*s. 2nd Edition. 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, 69469, 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.