INDIAN INSTITUTE OF TECHNOLOGY PATNA
DEPARTMENT OF CHEMISTRY

B.Tech in Chemical Science and Technology

Chemistry is central to the well being of the people and society. Chemistry has established itself as an integral part of natural Science and current applications of chemical science are impossible to ignore in virtually all industries. These include Petroleum, Healthcare & medicine, food and agriculture, polymer & synthetic materials, nanotechnology and others. In fact, the list is virtually endless. With a growing demand for dedicated expertise in different areas of Chemistry in industry and technology, it is understandable that industries are looking for scientists who can apply the science in developing their technology and scientists are showing inclination to hone their research to cater the technological demand of the industries.

A four year Bachelor of Technology (B.Tech) programme in Chemical Science and Technology is being proposed by the Department of Chemistry at IIT Patna from the year 2013. This program, as the name suggest, would promote Science as well as Technology involving Chemistry and other Chemistry related interdisciplinary areas. This program has been envisioned with a view to prepare human resource to be competent in both Academia and Industry. The scope of this program will extend by not limited to provide students with basic concepts of chemical science and in parallel offer adequate practical training in chemical science related engineering. This practice should enable the students to apply their theoretical concepts into a technological output whereby they can prove to be useful in industry for technology development.

The chemical science interface will develop the basic concepts of Organic, Inorganic, Physical and Biochemistry. From organic synthesis, Supramolecular chemistry to Thermodynamics and other aspects of chemistry, this part of the program will play a key role in developing the basic knowledge in chemistry along with the most updated findings in these areas. Thus, a solid academic platform for the students is foreseen with the science component of the program. Technological aspect of the program will include applied catalysis, drug design, medicinal chemistry, nanomaterials and nanoscience, fine and bulk chemicals, green chemical and technological practices.

The Department of Chemistry at IIT Patna continues to thrive to be a nationally-acclaimed model for educating and graduating students in Chemistry and related areas. We want our students to be prepared to compete in and contribute to the ever-changing, technology-centered world of the 21st century. To achieve this vision, the department is committed to providing a course of study for undergraduates in the chemical sciences and Technology which combines curriculum, high-quality teaching, innovative and intellectually challenging practical courses and employ state-of-the-art technologies.

The department of Chemistry is emerging as a strong contender in terms of achievement in chemical science and technology research with the support of a dynamic team consisting of teaching staff, non-teaching staff, project fellows and inspired research students. The continuously growing community in the department is sure to foster multi-disciplinary curriculum development to provide students with a breadth of course options in virtually all aspects of chemical science and related technology development. The students will be trained to do frontline research in interdisciplinary areas, which include materials science, environmental science and molecular biology.

Graduates from this program will have diverse job opportunities in the chemical industry, in petroleum industry including polymer and paint industry, pharmaceutical and healthcare industry, food industry, Biotechnology based industries, in environment related industries and businesses, and in Research & Development. Equally promising career in academics to pursue a research career in India and abroad seems appropriate also.

New technologies and the comfortable lifestyle enjoyed by us are provided through the applications of chemistry. Those who are deprived of the above, well being of them can be achieved through Chemical Science itself, be it a life saving drug or affordable synthetic materials for multipurpose applications. Sustainable improvement will only be achieved through public appreciation of the importance and positive aspects of chemical science and its related applications in technology in everyday life. The betterment of society covers three pillars: (1) Environment (2) Health and Safety and (3) Economy and Energy. We believe, the Chemical Science and Technology program at IIT Patna will contribute significantly to all the three issues and prepare graduates who can contribute to strengthen these pillars in our country.

Course Structure and Syllabus for B.Tech in Chemical Science and Technology

Semester - I

Course No	Course Name	L	T	P	C
CH101	Chemistry-I	3	1	0	8
EE101	Electrical Sciences	3	1	0	8
MA101	Mathematics - I	3	1	0	8
PH101	Physics - I	2	1	0	6
CH110	Chemistry Laboratory	0	0	3	3
ME110	Workshop – I	0	0	3	3
ME111	Engineering Drawing	2	0	3	7
HS101	English: Learning through Literature	3	0	0	6
		16	**4**	**9**	**49**

Semester-II

Course No	Course Name	L	T	P	C
CH102	Chemistry-II	3	0	0	6
CS 101	Introduction to Computing	3	0	0	6
MA102	Mathematics - II	3	1	0	8
ME101	Engineering Mechanics	3	1	0	8
PH102	Physics-II	2	1	0	6
CS110	Computing Laboratory	0	0	3	3
EE102	Basic Electronics Laboratory	0	0	4	4
PH110	Physics Laboratory	0	0	3	3
		14	**3**	**10**	**44**

Semester-III

Course No	Course Name	L	T	P	C
MA201	Mathematics - III	3	1	0	8
CS201	Object Oriented Programming and Data Structures	3	0	3	9
CB201	Chemical Process Calculations	2	1	0	6
ME 204/CBXXX	Fluid Mechanics-I	2	1	0	6
CH203	Organic Chemistry	3	1	0	8
CH205	Introduction to Quantum Chemistry	3	0	0	6
HS2xx	HSS Elective I	3	0	0	6
		19	**4**	**3**	**49**

Semester-IV

Course No	Course Name	L	T	P	C
CH202	Inorganic Chemistry	3	0	0	6
CH204	Polymer Chemistry	3	0	0	6
CH206	Medicinal Chemistry and Drug Discovery	3	0	0	6
CH208	Chemical Thermodynamics & Equilibrium	3	0	0	6
CH210	Chemical Technology Lab -I	0	0	6	6
HS2xx	HSS Elective II	3	0	0	6
XX2xx	Science Elective	3	0	0	6
		18	**0**	**6**	**42**

Semester-V

Course No	Course Name	L	T	P	C
ME305/CBXXX	Heat and Mass Transfer	3	1	0	8
CH301	Industrial Chemistry	3	0	0	6
CH303	Chemical Kinetics and Electrochemistry	3	0	0	6
CH305	Biochemistry and Biotechnology	3	0	0	6
CH307	Analytical Techniques in Chemistry	3	0	0	6
CH310	Chemical Technology Lab II	0	0	6	6
		15	**1**	**6**	**38**

Semester-VI

Course No	Course Name	L	T	P	C
CH302	Environmental Science and Technology	3	0	0	6
CH304	Petroleum and Petrochemicals	3	0	0	6
CB302	Chemical Reaction Engineering	3	0	0	6
CH306	Computational Chemistry	2	0	1	5
CH308	Dyes, Paints and Pigments	3	0	0	6
CH320	Chemical Technology Lab-III	0	0	6	6
HS3xx	HSS Elective	3	0	0	6
		17	**0**	**7**	**41**

Semester-VII

Course No	Course Name	L	T	P	C
CH400	Summer Training	0	0	0	2
CH401	Catalysis	3	0	0	6
CH4xx	Dept. Elective I	3	0	0	6
CH4xx	Dept. Elective II	3	0	0	6
XXxxx	Open Elective-I	3	0	0	6
CH410	Project - I	0	0	10	10
		12	**0**	**10**	**36**

Semester-VIII

Course No	Course Name	L	T	P	C
CH4xx	Dept. Elective -III	3	0	0	6
CH4xx	Dept. Elective- IV	3	0	0	6
CB406	Bio Process Engineering	3	0	0	6
XXxxx	Open Elective-II	3	0	0	6
HS4xx	HSS Elective	3	0	0	6
CH411	Project-II	0	0	16	16
		15	**0**	**16**	**46**

Total Credits = **345**

Syllabus

1st Semester and 2nd Semester all courses are common and existing. Hence syllabus is not provided here for those courses.

SECOND YEAR
3rd Semester

MA201 Mathematics-III 3-1-0-8

Already existing.

CB201 Chemical Process Calculations 2-1-0-6

Steady-state and dynamic processes; lumped and distributed processes; single and multi-phase systems; correlations for physical and transport properties; equilibrium relations; ideal gases and gaseous mixtures; vapor pressure; Vapor liquid equilibrium; Material balances: non-reacting single-phase systems; systems with recycle, bypass and purge; processes involving vaporization and condensation. Intensive and extensive variables; rate laws; calculation of enthalpy change; heat of reaction; fuel calculations; saturation humidity, humidity charts and their use; energy balance calculations; flow-sheeting; degrees of freedom and its importance in flow-sheeting.

Texts:

1. R. M. Felder and R. W.Rousseau, *Elementary principles of chemical processes*, 3rd Ed., Wiley, 1999.
2. D. M. Himmelblau, *Basic Principles and Calculations in Chemical Engineering*, 6th Ed., Prentice Hall of India, 2001.

References:

1. N. Chopey, *Handbook of Chemical Engineering Calculations*, 3rd Ed., Mc-Graw Hill, 2004
2. A. Olaf, K.M. Watson and R. A. R.Hougen, *Chemical Process Principles, Part 1: Material and Energy Balances*, John Wiley & Sons, 1968.

ME204/CBXXX Fluid Mechanics-I 2-1-0-6
Already existing.

CH203 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.

CH205 Introduction to Quantum Chemistry 3-0-0-6

The motivation for Quantum mechanics: 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 rotor, 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.

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.

HS2XX HSS Elective 3-0-0-6

Already existing.

4th Semester

CH202 Inorganic Chemistry 3-0-0-6

Acid-Base Chemistry: Definitions and concepts- Brønsted Lowry, Lux-Flood, Solvent system, Lewis, Usanovich, Hard-Soft Acid and Base (classification, strength and relation with electronegativity). Redox reactions and oxidation states, Reduction potentials and Gibbs energy, Disproportionation, Potential diagrams, Frost–Ebsworth diagrams, The effect of complex formation or precipitation on M^{2+}/M reduction potentials, Applications of redox reactions to industrial processes. Chemistry of

Boron (Hydrides, halides, Oxides, oxoacids, oxoanions and hydroxides), Chemistry of Silicon, Chemistry of Phosphorus (Oxides and oxoacids of P, Phosphazines). Halides, oxohalides, complex halides, oxides of Se, Te and oxoacids/salts, Interhalogen compounds and polyhalogen ions, Oxides and oxofluorides, Oxoacids and salts of Chlorine, Chemistry of Xenon.

Texts:

1. Catherine E. Housecroft, and Alan G. Sharpe, *Inorganic Chemistry*, Prentice Hall; Third edition, 2007
2. James E. Huheey, Ellen A. Keiter, Richard L. Keiter and Okhil K. Medhi, *Inorganic Chemistry: Principles of Structure and Reactivity*, Imprint: Pearson Education, First Edition, 2006.
3. D. J. Shriver, P. W. Atkins, and C. H. Langford, *Inorganic Chemistry*, 2nd Ed., ELBS ,1994.

Reference:

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

CH204 Polymer Chemistry 3-0-0-6

Basic Principles: Introduction and historical development, types of polymerization reaction, Nomenclature, Industrial polymers, Number and weight average molecular weights and their measurement techniques, Viscometry, molecular weight distribution. Chemical structure and polymer morphology: Amorphous state and crystallinity, Glass transition temperature, stereochemistry, crosslinking, polymer blends. Chemical structure and polymer properties: Thermal stability, mechanical properties, flammability, chemical resistance, degradability and electrical conductivity. Free radical polymerization: Introduction, free radical initiators, kinetics, mechanism and stereochemistry. Ionic polymerization: cationic and anionic polymerization - kinetics, mechanism and stereochemistry. Transition metals in polymerization: Ziegler-Natta polymerization and Metathesis polymerization

Texts:

1. Malcolm P. Stevens, *Polymer Chemistry: An Introduction*, Oxford University Press, USA, Third Edition, 1998
2. Robert J. Young, and Peter A. Lovell, *Introduction to Polymers*, CRC Press, Third Edition, 2011

References:

1. Paul C. Hiemenz, and Timothy P. Lodge, *Polymer Chemistry*, CRC Press, Second Edition, 2007.

CH206 Medicinal Chemistry and Drug Discovery 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.

CH208 Chemical Thermodynamics and Equilibrium 3-0-0-6

Ideal gases, real gases, critical state; thermodynamic laws; reversible and irreversible processes; Thermochemistry: Hess's law, Kirchoff's equation; Joule-Thompson Experiment and Co-efficient, 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; The thermodynamic description of mixtures, 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.

Texts:

1. G. W. Castellan, *Physical Chemistry*, 3rd Ed., Addison Wesley Publishing Company, 1983.
2. P. W. Atkins, and J. de Paula Atkins, *Physical Chemistry*, 7th Ed., Oxford University Press, 2002.
3. A Textbook of Physical Chemistry, K.L Kapoor, 4th Edition, MacMillan Publishers, India Ltd.

CH210 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.

Text:

J. R. Mohrig, T. C. Morrill, C. N. Hammond and D.C. Neckers, *Experimental organic chemistry*, W.H. Freeman and Co. ,1998.

References:

1. N. K. Vishnoi, *Advanced practical organic chemistry*, Vikash publishing house Pvt. Ltd., 1996.
2. 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.

HS2XX HSS Elective-II 3-0-0-6
Already existing.

XX2XX Science Elective 3-0-0-6
Already existing.

Third Year

5th Semester

ME305/CBXXX Heat and Mass Transfer 3-1-0-8

Already existing.

CH301 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.

Texts:

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

References:

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

CH303 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.

CH305 Biochemistry and Biotechnology 3-0-0-6

Molecular components of cells: Proteins-3d conformation, lipids & membranes, sugars & storage polysaccharides, nucleotides-3d structure, vitamins and coenzymes. Catabolic and anabolic pathways: Oxidative degradation of fatty acids & amino acids; electron transport and phosphorylation; Biosynthesis of carbohydrates, lipids, amino acids & nucleotides. Biochemistry and origin of life:Transcription, translation, genetic code, gene expression and regulation, morphogenesis. Recombinant DNA technology:Polymerase Chain reaction, Gene manipulation for therapy, Genetically modified organisms (GMO), therapeutic proteins from GMOs; SNP, VNTRs, DNA vaccines, Antisense technology; microarrays; genomic and cDNA libraries. *Different aspects of Biotechnology:* Biotechnology processes for oil recovery (microbial), toxic wastes treatment, petroleum wastes treatment etc.; Biofuels: energy recovery systems for urban waste, technology evaluation, alcohol production from organic wastes; Biotechnology-derived Drug Products: Formulation Development, Stability Testing, Filling, and Packaging. Biosensors-Biocatalysts based, bio affinity based biosensors & microorganisms based biosensors, types of membranes used in biosensor constructions, applications of biosensors.

Texts:
1. Principles of Biochemistry, David Lee Nelson, Albert L. Lehninger, Michael M. Cox – 2008, W H Freeman Limited
2. Biotechnology, B. D. Singh, 2010, Kalyani Publishers

References:
1. Biochemistry, Jeremy M. Berg, John L. Tymoczko, Lubert Stryer, W H Freeman Limited
2. Basic Biotechnology -2nd Ed., Colin Ratledge and Bjorn Kristiansen, Cambridge University Press.

CH307 Analytical Techniques in Chemistry 3-0-0-6

Infrared spectroscopy: instrumentation and application in chemistry. Vibrations of polyatomic molecule, group frequency and its application, Electronic Spectroscopy: General principles and instrumentation, analytical applications: qualitative and quantitative analysis of inorganic and organic compounds. Nuclear magnetic resonance Spectroscopy: General principles, sensitivity of the method, Instrumentation. Application in chemical analysis (with special reference to 1H – NMR): basic definitions, shift reagents, off-resonance decoupling, multinuclear NMR. Mass spectrometry: theory and principles, Instrumentation, Methods of ionization. Structure elucidation of inorganic and organic compounds. Thermal Analysis (TGA and DSC) and its application in chemistry.

Texts:
1. D. L. Pavia, G. M. Lampman, G. S. Kriz, Introduction to Spectroscopy, 3rd edition, Thomson Brooks/Cole, (2000)
2. William Kemp, Organic Spectroscopy, 3rd edition, W.H. Freeman & Company, (1991).
3. R. M. Silverstein, G. C. Bassler, C. Morril, Spectrometric Identification of Organic Compounds, 5th edition, John Wiley & Sons, (1991)
4. 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.

References:
1. R. S. Drago, Physical Methods for Chemists, 2nd edition, Saunders College Publishing, (1992)
2. A. B. P. Lever, Inorganic Electronic Spectroscopy, 2nd edition, Elsevier, (1986)
3. K. Nakamoto, Infrared and Raman Spectra of Inorganic and Coordination Compounds, Part A & B, 5th edition, John Wiley & Sons Ltd., (1997)

4. M. Rose and R. A. W. Johnston, Mass Spectrometry for Chemists and Biochemists, 2nd edition, Cambridge University Press, (1996)

CH310 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. Engineering

Texts:

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.

References:

1. A. J. Elias, *A Collection of Interesting General Chemistry Experiments*, Revised Ed., Universities Press (India) Pvt. Ltd, 2007.
2. K. Hutchings, *Classic Chemistry Experiments*, The Royal Society of Chemistry, London, 2000

6th Semester

CH302 Environmental Science and Technology 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.

CH304 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.

CB302 Chemical Reaction Engineering 3-0-0-6

Classification of chemical reactions; single, multiple, elementary and nonelementary homogeneous reactions; order and molecularity; temperature dependency; constant and variable volume batch reactor; reaction rate; rate constant; collection and interpretation of kinetic data; parallel and series reaction; batch, ideal plug flow and CSTR reactor design with and without recycle; temperature and pressure effects; Residence Time Distribution.

Texts:

1. H. S. Fogler, Elements of Chemical Reaction Engineering, Prentice Hall, 2nd Ed., New Jersey, 1992.
2. O. Levenspiel, Chemical Reaction Engineering, 2nd Ed., Wiley Eastern, 1972.

Reference:

1. J. M. Smith, Chemical Engineering Kinetics, 3rd Ed., McGraw Hill, 1980.

CH306 Computational Chemistry 2-0-1-5

Wavefunction of a particle in a box, harmonic oscillator, anharmonic oscillator, r-dependent wavefunction of a hydrogen atom, atomic & hybridized orbitals, Wein's Law, Ionization energy of hydrogen, Time dependent Perturbation theory: , Integration of Schrodinger Equation: 1D box, spherical box, simple harmonic oscillator, Eigen Values and Eigen Vectors, SCF energies and dipole moment, Calculation of auto-correlation function Fourier Transform and Spectral Applications.

Texts:

1. R. D. Levine, *Molecular reaction dynamics*, C.U.P., Cambridge, 2005.

References:

1. W. H. Press, *Numerical recipes: the art of scientific computing*, 3rd Ed., C.U.P., Cambridge, 2007.
2. W. Gehrke, *Fortran 95 language guide*, Springer Verlag, London, 1996.
3. S. A. Rice and M. Zhao, *Optical control of molecular dynamics*, John Wiley & Sons, New York, 2000.

4. H. D. Meyer, F. Gati and G. A Worth, *Multidimensional, quantum dynamics: MCTDH theory and applications*, John Wiley, 2009.

CH308 Dyes, Paints and Pigments 3-0-0-6

Paints: Compositions binders, extender, thinner and surface active agents; functions of the ingredients; Paint formulations; Importance of PVC, alkyds, epoxy and polyurethane resins. **Pigments:** Introduction – Requirements of a pigment, typical 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. **Dyes:** Colour and chemical constitutions; classification; brightening agents; cyanine dyes; chemistry of colour developer – instant colour processes; synthesis and applications of methyl Orange, congo red, crystal violet, malachite green, phenolphthalein, fluorecein, alizarin and Indigo and Rhodamine B etc. phenolphthalein, fluorecein, alizarin and Indigo.

Texts/References:
1. Samuel Delvin, *Dyes and Pigments*, Ivy Publishing House, 1st Ed. 2006
2. W. Hebst,K. Hunger, *Industrial Organic Pigments*, Wiley-VCH, 3rd Edition

CH320 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 sound velocity in liquids systems. Experiments based on EMF and conductance measurements: determination of electrode potentials, solubility product, pH equivalent conductance; Determination of the CMC of surfactants from Conductivity and Surface Tension Measurements, Equilibrium: Adsorption of an Organic Acid by Activated Carbon in Aqueous Media using the Langmuir Adsorption Isotherm and determination of surface area; Experiments based on phase equilibria: Study of binary and ternary liquid systems; Measure the rate constant for electron transfer by quenching using Stern-Volmer equation.

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.

HS3XX HSS Elective 3-0-0-6
Already existing.

7th Semester

CH400 Summer Training 0-0-0-2

CH401 Catalysis 3-0-0-6

The basics of catalysis. Different types of catalysts. Homogeneous and Heterogeneous catalysis. Freundlich adsorption isotherm, Langmuir adsorption isotherm, determination of surface area of adsorbent, BET adsorption isotherm, thermodynamic treatment of adsorption, adsorption at the surface of a liquid. Biocatalysis, design and developing industrial catalysts: preparation of catalysts; characterization of catalysts; Practical examples of catalysts. Organocatalysis, enzymatic catalysis, transition metal catalysis etc.

Texts:

1. Gadi Rothenberg, Catalysis: Concepts and Green Applications, 1st Ed. Wiley-VCH, 2008.
2. K. L. Kapoor, Text Book of Physical Chemistry, Vol 5, 2nd Edition, Macmillan Publisher Ind. Ltd

References:

1. J. J. Carberry, Chemical and Catalytic Reaction Engineering, Dover, 2001.
2. J. Weitkamp, and L. Puppe (eds.), Catalysis and Zeolites: Fundamentals and Applications, Springer Verlag, 1999.

CH4XX Dept. Elective I 3-0-0-6
CH4XX Dept. Elective II 3-0-0-6
XX4XX Open Elective-I 3-0-0-6
CH410 Project-I 0 -0-10-10

8th Semester

CH4XX Dept. Elective II 3-0-0-6
CH4XX Dept. Elective IV 3-0-0-6
CB406 Bio Process Engineering 3-0-0-6

Introduction to Bioprocesses : Traditional and modern bioprocess Engineering-overview, integrated bioprocess, upstream and downstream operations, process flow sheets; Material balance and Energy balance for different systems; Stoichiometry of cell growth and product formation; Energetic analysis of microbial growth and product formation; thermodynamic efficiency of growth, Enzyme technology- Enzyme kinetics, immobilization and industrial production. Fermentation Processes: Fermentation processes-outline, overview & types, design, parameteres & construction of fermentor and ancillaries; application in the biotechnology industry; kinetic models for microbial growth; behavior of microbes in different reactors; Media design: requirements for fermentation processes and optimization techniques (placket Burman Design). Separation technology : Solids removal operations - settling, centrifugation and filtration; Product isolation - adsorption and extraction; Purification techniques - precipitation, ultrafiltration, chromatography and electrophoresis; Product polishing operations- crystallization and drying; Integrated bio-reaction and bio-separation processes- membrane bioreactors, extractive fermentation. Bioprocess Engineering and Industry:
Environmental biotechnology - wastewater engineering, bioremediation; Bioprocess instrumentation; Biological systems for the production of commercial goods and services: foods, feed, pharmaceuticals, nutraceuticals, chemicals, polymers, fuels, equipment, diagnostics and other biomaterials; good manufacturing practices, Safety and regulatory issues.

Text:
1. *Bioprocess Engineering Basic Concepts*, Michael L. Shuler and Fikret Kargi, Prentice Hall PTR.

Reference:
1. *Bioprocess Engineering Principles*, Pauline M. Doran, Academic Press.

XX4XX	**Open Elective-II**	**3-0-0-6**
HS4XX	**HSS Elective**	**3-0-0-6**
CH411	**Project-II**	**0-0-16-16**

List of Departmental Electives

Semester-VII

CH403 Group Theory & Spectroscopy 3-0-0-6

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; Molecular Spectroscopy: Energy levels, MO, vibronic transitions, Franck-Condon principle, electronic spectra of polyatomic molecules; Microwave: classification of molecules, selection rules, intensity of spectral lines, effect of isotopic substitution; 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.

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

References:
1. M. Tinkham, *Group Theory and Quantum Mechanics*, McGraw Hill, 1964.
2. G. M. Barrow, *Introduction to Molecular Spectroscopy*, McGraw Hill, 1962.
3. H. E. White, *Introduction to Atomic Spectra*, McGraw Hill, 1934.

CH 405 Material Chemistry 3-0-0-6

Introduction to Materials Chemistry. Materials for Solid State Devices: Rectifiers, transistors, capacitors - IV-V compounds - low-dimensional quantum structures, optical properties, Nonlinear Optical Materials: Nonlinear optical effects, second and third order - molecular hyperpolarisability and second order electric susceptibility - materials for second and third harmonic generation. Polymeric Materials: Molecular shape, structure and configuration - crystallinity - streestrain behavior - thermal behavior - polymer types and their applications - conducting and ferroelectric polymers.

Liquids Crystals: Mesmorphic behavior - thermotropic and lyotropic phases - description of ordering in liquid crystals, the director field and order parameters - nematic and semectic mesophases, smectic -nematic transition and clearing temperature - homeotropic, planar and twisted nematics - chiral nematics - smectic A and smectic C phases - cholesteric-nematic transition - optical properties of liquid crystals - effect of external field.

Texts:

1. Malcolm P. Stevens, *Polymer Chemistry: An Introduction*, Oxford University Press, USA, Third Edition, 1998
2. Robert J. Young, and Peter A. Lovell, *Introduction to Polymers*, CRC Press, Third Edition, 2011
3. W.D. Callister, Material Science and Engineering. An Introduction, Wiley, New York (1985).

References:

1. Paul C. Hiemenz, and Timothy P. Lodge, *Polymer Chemistry*, CRC Press, Second Edition, 2007.
2. H.V. Keer, Principles of the Solid State, Wiley Eastern (1993).
3. N.W. Ashcroft, N.W. Mermin, Solid State Physics, Saunders College, Philadelphia (1976).

CH407 Advanced 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 dinitrogen compounds; 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 409 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.

CH501 Nanobiotechnology 3-0-0-6

Already existing M.Tech elective course

Semester-VIII

CH 402 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.

CH512 Nanotechnology for Medical Diagnostics and Therapy 3-0-0-6

Already existing M.Tech elective course

CH404 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; 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 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.

CH406 Colloids and Surface Chemistry 3-0-0-6

Colloidal state of matter. Properties of lyophillic and lyophobic colloidal solutions. Thermodynamics of electrified interface, stability of colloidal solutions: Theory of Verwey and Overbeek, colloidal electrolytes, polyelectrolytes. Donnan membrane equilibria. Determination of molecular weight of macromolecules. Micelles, reverse micelles. Surface energetics and adsorption from liquids. Emulsion, detergent, gels and foams. Applications in detergents, personal-care products, pharmaceuticals, nanotechnology, and food, textile, paint and petroleum industries.

Texts/References:

1. P. C. Hiemenz and R. Rajagopalan, *Principles of Colloid and Surface Chemistry*, Marcel Dekker, New York, 1997.
2. J. C. Berg, *An Introduction to Interfaces and Colloids: The Bridge to Nanoscience*, World Scientific, Singapore, 2010.
3. P. Ghosh, *Colloid and Interface Science*, PHI Learning, New Delhi, 2009.
4. A. W. Adamson and A. P. Gast, *Physical Chemistry of Surfaces*, John Wiley & Sons, New York, 1997.
5. J. Israelachvili, *Intermolecular and Surface Forces*, Academic Press, New York, 1992.
6. R. J. Hunter, *Foundations of Colloid Science*, Oxford University Press, New York, 2005.

CH502 Supramolecular Chemistry 3-0-0-6
Already existing M.Tech elective course

CH511 Theory and Modelling in Nanoscience 3-0-0-6
Already existing M.Tech elective course