

INSTITUTE OF CHEMICAL TECHNOLOGY – IOC Bhubaneswar
(University under Section 3 of UGC Act 1956, Elite Status & Centre of
Excellence – Government of Maharashtra)
DEPARTMENT OF CHEMISTRY

M.Sc (Chemistry)
Proposed Revision of Syllabus 2023
(as per NEP 2020 recommendations)

Regulations and Syllabus relating to the Degree of Master of Science in Chemistry
(M. Sc. Chemistry)

A. Preamble

Chemistry is a fundamental science what connects us to the world. Concomitant to the developments in other fields of science, the developments in Chemistry are taking place at a phenomenal pace. Chemistry overlaps with many other disciplines in science and these developments bring out this aspect profoundly.

The current M.Sc. Chemistry program offered by the Department of Chemistry, ICT (Mumbai campus) aims to equip the students with a lucid understanding of the basic concepts while introducing them to the latest cutting-edge developments in the field. The program is designed to approach the study of Chemistry as an interdisciplinary field of specialization. The program is not compartmentalized as Inorganic Chemistry, Organic Chemistry, Physical Chemistry, etc but aims to include a well-balanced learning of all critical aspects of the subject. The Institute of Chemical Technology, with advantage of having expertise in various aspects of Chemical Engineering and Chemical Technology, is an appropriate Institute to run such a program.

The current syllabus introduces the important aspects of the National Education Policy 2020 and the courses are revised to ensure that the content is up-to-date with the latest developments. The syllabus has been revised to offer exit option at the end of the first year and the concept of academic bank of credits. The program has the following special features:

- (1) The 2-year program includes a total of 88 credits distributed equally among the four semesters (22 credits per semester) which will be offered to students completing a 3-year undergraduate degree program with Chemistry as the major subject.
- (2) Students who have joined the two-year Master's degree program may opt for exit at the end of the first year and earn a PG Diploma.
- (3) The PG Diploma may be awarded to a student provided they have earned the requisite credits in one year including on-the-job training of 04 credits during summer break, after completion of the second semester of the first year in the respective major subject.
- (4) Re-entry to complete the PG degree, after taking the exit option, will be permissible up to 05 years from the date of admission to the PG program.
- (5) In addition to the theory and laboratory courses, the students will be expected to complete the research project in the second year of the Masters' program (4 credits in Semester III and 6 credits in Semester IV) in order to be awarded the PG Degree.
- (6) The assessment norms of the program will be in accordance to the NEP recommendations and prescribed by the Institute.
- (7) The ratio of in-semester and end-semester assessment marks shall be 50:50. In the end-semester assessment there will be a formal examination. In the in-semester assessment, there will be one formal midsemester examination carrying 30% marks. In addition, there will be a series of tests, assignments, presentations, quizzes as continuous assessment components, totally carrying 20% marks.
- (8) The assessment of the students shall be as per the norms of the Institute. Various activities associated with the semesters will be carried out as per the academic

calendar of the Institute. The requirement of attendance of the students shall be as per the norms of the Institute.

- (9) All the relevant academic Rules and Regulations of the Institute shall be applicable to the program. In case of any difficulty regarding any assessment component of the program, the Departmental Committee shall take appropriate decision, which will be final and binding.

1. Intake

30 candidates shall be admitted every year. The distribution of seats shall be as per the Institute's norms prescribed at the time of admission.

2. Admission and Eligibility

The admission to MSc (Chemistry) program in the ICT Mumbai campus shall be **strictly on the basis of merit in the entrance examination** conducted by the Institute. In order to be eligible for admission to the program, a candidate must fulfil the following criteria:

- (1) The candidate must have passed the post-H.S.C. 3-year degree course (Bachelor of Science) with Chemistry as a major subject (48 credits or equivalent). The B.Sc. degree shall be of any recognized University.
- (2) The candidate must have completed Mathematics courses at the H.S.C. level. If mathematics is not taken at the H.S.C. level, it must be one of the subjects taken at the B.Sc. level.
- (3) The candidate must have passed the B.Sc. degree with at least 60% of the marks in aggregate or equivalent grade average. [55% for the backward class candidates belonging to the state of Maharashtra] are only eligible to apply.
- (4) The candidates shall have cleared the B.Sc. degree examination in one attempt; i.e. candidates passing the B.Sc. degree in compartments shall not be eligible for the admission.

3. Program structure

The important points regarding the structure of the 2-year (four-semester) MSc Chemistry program are as follows:

- (1) Each semester will incorporate 16 weeks of instruction and there will be 22 credits for each semester.
- (2) A 4-credit Research Methodology course is compulsory in the first semester of the program.
- (3) **Electives: One elective to be offered per semester.** The electives to be offered during a given semester will be declared by the Head of Department before the commencement of the semester. Any elective course, in addition to those mentioned in the current syllabus, may be offered to the students after due approval.
- (4) **Internship / Field project:** Completion of internship or field project is a compulsory criterion for awarding the PG Diploma or the PG degree. The field project / internship should be of a minimum duration of 4 weeks and will be schedule after semester 2 and before commencement of semester 3. The assessment of the field project / internship will be as per the prescribed format.
- (5) **Project:** At the end of the second semester, the Head of Department will assign the supervisors for the project. The students will do the experimental work on the project and submit the thesis before the prescribed date, which will be a date before the last date of the semester IV. The thesis shall be submitted in the format prescribed. The thesis will be evaluated by the supervisor along with one other external referee as per the norms.

SEMESTER I

Course No.	Title	h/ week	Credits	Marks
CHT 3002	Organic Reaction Mechanism	4	4	100
CHT 3004	Chemical Dynamics	4	4	100
CHT 3005	Instrumental Methods of Analysis	4	4	100
HUT 3102H	Research Methodology	4	4	100
CHT XXXX	Elective paper – 1	4	4	100
CHP 3002	Organic Chemistry Laboratory	4	2	100
			22	

SEMESTER II

Course No.	Title	h/ week	Credits	Marks
CHT 3007	Chemistry of Transition Metals	4	4	100
CHT 3009	Molecular Thermodynamics	4	4	100
CHT 3033	Stereochemistry and Spectroscopy of Organic Compounds	4	4	100
CHT XXXX	Elective paper – 2	4	4	100
CHP 3008	Inorganic and Instrumental Chemistry Laboratory	4	2	100
CHT 3009	Internship / Field project	4	4	100
			22	

SEMESTER III

Course No.	Title	h/ week	Credits	Marks
CHT 3003	Heterocyclic Chemistry	4	4	100
CHT 3006	Quantum Chemistry	4	4	100
CHT 3011	Organic Synthesis	4	4	100
CHT XXXX	Elective paper – 3	4	4	100
CHP 3010	Physical and Computational Chemistry Laboratory	4	2	100
CHP 3011	Research project – 1	4	4	100
			22	

SEMESTER IV

Course No.	Title	h/ week	Credits	Marks
CHT 3010	Radicals, photochemistry and pericyclic reactions	4	4	100
CHT 3015	Solid State Chemistry and Group Theory	4	4	100
CHT 3034	Organometallic Chemistry and Catalysis	4	4	100
CHT XXXX	Elective Paper – 4	4	4	100
CHP 3012	Research project – 2		6	200
			22	

Total Credits: 88

Elective Papers

CHT 3013	Industrial Chemistry
CHT 3016	Biochemistry
CHT 3018	Chemistry of Main Group Elements
CHT 3021	Natural Products
CHT 3022	Polymer Chemistry
CHT 3023	Surface and Interfacial Chemistry
CHT 3024	Computational Chemistry
CHT 3025	Nuclear Chemistry
CHT 3026	Bioinorganic Chemistry
CHT 3027	Developments in Organic Synthesis
CHT 3028	Supramolecular Chemistry
CHT 3029	Materials Chemistry
CHT 3030	Separation Processes
CHT 3031	Green Chemistry
CHT 3032	Material and Energy Balance

SEMESTER I

	Course Code: CHT 3002	Course Title: Organic Reaction Mechanism	Credits = 4		
	Semester: I	Total contact hours: 60	L	T	P
			3	1	0
Course Outcomes (Students will be able to.....)					
1	Identify the important reactive intermediates and list their properties				
2	Discuss the various reaction mechanisms and the influence of various factors on the mechanism				
3	Estimate the plausible reaction mechanism and the experimental methods to verify the same				
4	Evaluate the mechanistic details involving different reactive intermediates based on properties of reacting molecules				
List of Prerequisite Courses					
	Undergraduate course on Organic Chemistry				
Course Contents (Topics and subtopics)					
			Reqd. hours		
1	Organic reactive intermediates: Generation, stability, and reactivity of carbocations, carbanions, free radicals, carbenes, and nitrenes. Non-classical carbocation, neighbouring group participation				6
2	Nucleophilic Substitution at Saturated Carbon: Mechanism and Stereochemistry of S _N 1, S _N 2, S _N i and S _N 2' reactions. Reactivity: The effect of substrate structure, attacking nucleophile, leaving group, and reaction medium. Phase transfer catalysis, Ambient nucleophiles: Regioselectivity. Competition between S _N 1 and S _N 2 mechanisms.				8
3	Elimination reactions: Elimination: E1, E2, E1cB, Zaitsev and Hoffmann elimination, orientation in elimination reactions, energy profile diagrams, the effect of the structure of the substrate, base, solvent etc.				6
4	Addition reactions to C-C multiple bonds: Electrophilic additions to alkenes and alkynes, energy profile diagrams, Markovnikov's addition.				5
5	Acid-Base concept: pK _a values, acid strength, tautomerism - including ring-chain and valence tautomerism, Chemistry of enolates, reactions of enolates, thermodynamic and kinetic control				5
6	Methods of determining reaction mechanism: Trapping of intermediates, cross-over experiments, isotopic effect and labeling, stereochemical studies, kinetic effect, Salt effect, Energy profile diagrams, Concept of transition state and reaction coordinate.				6
7	Frontier molecular orbital theory and its applications.				5
8	Study of reactions: Prins, Neber, Nef reaction, Hoffman reaction, Wagner-Meerwein reaction, Julia olefination, Peterson olefination, Corey-Winter, Corey-Fuchs, etc.				5
9	Esterification and hydrolysis of esters: Mechanisms involving acid-catalyzed and base catalyzed hydrolysis.				4
10	Aromaticity: Benzenoid and non-benzenoid compounds, Huckel's molecular orbital theory, Frost-Muslin geometrical interpretation, antiaromaticity, Application to carbocyclic and heterocyclic systems, annulenes, azulenes. Reactions of aromatic compounds: Aromatic electrophilic and nucleophilic substitution, benzyne intermediate, aromatic substitution reactions involving radical intermediates				10
List of Text Books					
	Organic Chemistry—by J. Clayden, N. Greeves, S. Warren and P. Wothers (Oxford)				
	Advanced Organic Chemistry: Part A and B: Francis Carey				

	Advance Organic chemistry, Reinhard Bruckner, Elsevier	
	A guidebook to mechanism in organic chemistry – Peter Sykes 6th Ed.	
	Organic chemistry- R. T. Morrison and R. N. Boyd,(Prentice Hall.)	
	Organic Chemistry Vol. I (Sixth Edn.) and Vol. II (Fifth Ed.,) by IL Finar ELBS	
List of Additional Reading Material / Reference Books		
	Advanced Organic Chemistry –by J. March 6th Edition	
	Organic reaction mechanism (Benjamin) R. Breslow	
	Mechanism and structure in Organic Chemistry – E. S. Gould	
	Modern Organic Reaction Mechanism: G. Whitmore: Sarup and Sons Publishers and distributors	

	Course Code: CHT 3004	Course Title: Chemical Dynamics	Credits = 4		
	Semester: I		Total contact hours: 60	L	T
			3	1	0
Course Outcomes (students will be able to.....)					
1	Express the rate laws for different mechanisms using appropriate models				
2	Apply the rate laws to chemical reactions and processes				
3	Evaluate the kinetic model by comparing the experimentally observed data with the proposed rate law				
4	Analyze the kinetic aspects of chemical processes taking place on the interfacial electrode surface				
5	Compare the theoretically predicted rates with the rates computed experimentally				
List of Prerequisite Courses					
	Undergraduate Physical Chemistry course				
Course Contents (Topics and subtopics)					
			Reqd. hours		
1	Introduction – rate law, order and molecularity, mechanism				3
2	Kinetics of parallel, reversible and consecutive reactions				4
3	Kinetics and reaction mechanism – steady state and rate determining step				4
4	Mechanism of thermal / photochemical chain reactions				4
5	polymerization reactions				3
6	Chain reactions, branched chain reactions and explosion limits				4
7	Kinetics of homogeneous acid / base catalyzed reactions				3
8	Enzyme Catalysis – Michaelis Menton mechanism, inhibition of enzymes				5
9	Electrode Kinetics: Electrical double layer, overpotential and its types, current density for single step and multi-step processes, Influence of electrical double layer on rate constants, Activation and diffusion controlled processes- Marcus kinetics,				6
10	Butler-Volmer equation and its implications, Tafel plot				4
11	Kinetics of electrode reactions – One and two electron transfer reactions Mechanism of hydrogen evolution and oxygen reduction in acid and alkaline media. Experimental methods for elucidation of reaction mechanism.				7
12	Theories of reaction rates – Collision theory, transition state theory Solvent effects and diffusion controlled reactions				7
13	Reactions in molecular beams				4
14	Experimental techniques for measuring kinetics of fast reactions				2

List of Text Books	
Chemical Kinetics – K.J. Laidler	
Principles of Chemical Kinetics- J.C.House, C.Brown	
Modern Electrochemistry- J.O.M. Bockris and A.K.N. Reddy- Volumes I and II	

Course Code: CHT 3005	Course Title: Instrumental Methods of Analysis	Credits = 4		
		L	T	P
Semester: I	Total contact hours: 60	3	1	0

Course Outcomes (students will be able to.....)

1	Describe the principles and applications of various instrumental techniques	
2	Compare the results from various analytical techniques for gaining information about samples	
3	Modify the existing procedures and protocols to improve sensitivity, selectivity and accuracy of the analysis	
4	Develop analytical protocols using various methods to carry out sample analysis	

List of Prerequisite Courses

Undergraduate Analytical Chemistry	

Course Contents (Topics and subtopics)

		Reqd. hours
1	Basics Theory: Statistical and mathematical operations in Chemistry, Units, dimensions and concentration, Errors and evaluation, Solid Sampling. Precision and Accuracy, Deviations, T- F- and Q-tests, Grubb's test, Regression analysis, Instrument calibration and validation.	10
2	Flame absorption and emission spectrometry: Theory, sources, burners, atomic emission spectra, atomic absorption spectra, effect of temperature on emission, absorption and fluorescence, electro thermal atomizers, Instrumentation for FES, radiation sources atomic absorption methods, instrumentation for AAS, spectral interferences, standard addition and internal standard method of analysis, comparison of atomic absorption and emission methods, inductively coupled plasma, Applications of AAS, AES and ICPAES,	12
3	Molecular luminescence: Introduction, Fluorescence, photo luminescent theory (Jablonski Diagram), electron transitions during photoluminescence, factors affecting photoluminescence, luminescent apparatus, optical extractive sources, wavelength selectors, detectors and readout devices, photo luminescent spectra, photo luminescent analysis, analysis of non-photoluminating compounds, specific examples of analysis using photoluminescence, Applications.	6
4	Chromatography: GC and HPLC-Principles, columns including chiral columns, detectors. Ion exchange chromatography, exclusion chromatography, gel permeation chromatography,	10
5	Hyphenated Techniques: GC-MS, LC-MS, HP-TLC Basic principles, Analysis of vacuum and gas flow, Interfaces, Computerization, Computerized operation, Characteristics, Data analysis	6
6	Electroanalytical method: voltametry, cyclic voltametry, coulometry, ion selective electrodes and sensors, polarography, anodic/cathodic stripping, electroless deposition	10
7	Diffraction techniques: Powder X-ray diffraction methods. Principle (Braggs law), Theory- X-ray spectral lines, X-ray tube, X-ray emission, Absorptive apparatus: Sources, Collimation, sample handling, wavelength	6

	dispersive devices, Energy dispersive devices, detectors, readout device, sample analysis using XRD	
List of Text Books		
	Skoog, Holler, Crouch, West - Fundamentals of Analytical Chemistry	
	David Harvey-Modern Analytical Chemistry	
	Quantitative Analysis, sixth edition- R.A. Day, A. L. Underwood	
List of Additional Reading Material / Reference Books		
	Pollard S.J.T., Thompson F. E., McConnachie G.L.-Ion Exchange Chromatography (1995)	
	Basics Gas Chromatography, Harold M. McNair, James Miller	
	Basic Gas Chromatography Mass Spectrometry, Principles and Techniques, F.W. Karasek and R.E. Clement, Elsevier, (Elsevier Science B.V.) 1988	
	Introduction to Instrumental Analysis by R. D. Broun, Mc Graw Hill (1987)	
	Instrumental methods of chemical analysis by H. Willard, L. Merrit, J.A. Dean and F.A. Settle. Sixth edition CBS (1986)	

	Course Code: HUT 3102H	Course Title: Research Methodology	Credits = 4		
	Semester: I		Total contact hours: 60	L	T
			3	1	0
Course Outcomes (students will be able to.....)					
1	Understand the fundamental aspects of undertaking a research project				
2	Develop relevant and lucid outline of a research problem with clear objectives				
3	Design and optimize the methods aimed at solving a given research problem				
4	Understand and implement the various skills of scientific data analysis				
5	Make use of modern tools for effective communication of results				
List of Prerequisite Courses					
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	Course Contents (Topics and subtopics)				Reqd. hours
1	Nature of Science, scientific enquiry, and scientific method. Theory, law, hypothesis, prediction				4
2	Nature of Chemistry, Chemical research – Types, process. Defining and addressing of research problem, Research hypothesis. Creative problem solving				4
3	Chemical literature survey: Chemical nomenclature systems, Introduction to library, Types of resources available including online resources, Introduction to Chemical Abstracts, Effective use of resources, Compilation of references, Critical review of literature				8
4	Methods in Chemical research: Selection of Problem, Experimental conditions, use of solvents, catalysts, temperature, pressure etc, Scientific instruments: Least count, calibration, sensitivity, resolution, validation.				10
5	Scientific data: 4.1 Variables – controlled, dependent, independent. SI units. Significant figures				8

	4.2 Accuracy, precision, reproducibility. Uncertainty in measurements – components of uncertainty. errors 4.3 Organization and presentation of data, Graphical communication, Powerpoint presentations	
6	Writing of - Research paper, PhD thesis, Research project. Scientometry.	6
7	Intellectual property issues: Confidential data, patent, copyrighted material, trade mark, etc, effective record keeping, Writing Patents	6
8	Responsible conduct of research: Responsible decision-making, ethical issues, Plagiarism and Similarity	4
9	Quality, TQM, GLP	4
10	Safety in Chemical research	6
List of Text Books		
	Research Methodology – Methods & Techniques, C.R. Kothari, Wiley Eastern Ltd, New Delhi 1985.	
	Research Methodology – A Step by step Guide for Beginners 2nd edn Kumar Ranjit, Pearson Education, Singapore, 2005.	
	Practical Research Methods, Catherine Dawson, UBS Publisher's Distribution, New Delhi 2002.	
	Introduction to Research & Research Methodology M. S. Sridhar	

Elective Paper I CHT XXXX

Practicals:

	Course Code: CHP 3001	Course Title: Organic Chemistry Laboratory	Credits = 2		
			L	T	P
	Semester: I	Total contact hours: 60			4
Course Outcomes (students will be able to.....)					
1	Perform one-step and two-step synthetic procedures for organic compounds				
2	Choose an appropriate separation technique to isolate the product				
3	Analyze the product and determine the purity of the same				
4	Optimize the synthetic methods to improve yield and selectivity				
List of Prerequisite Courses					
	Undergraduate Organic Chemistry laboratory course				
Course Contents (Topics and subtopics)					
					Reqd. hours
1	Purification techniques: Crystallization, distillation – simple and fractional, sublimation, steam distillation, chromatography – TLC and column. Purity checking through physical constants and TLC.				40
2	Separation techniques: Separation of multicomponent mixtures through Physical and chemical methods				20
3					
List of Text Books					

	Vogel's Textbook of Practical Organic Chemistry, 5e, Arthur Vogel, Pearson India (2003)	
	Practical Organic Chemistry, by Mann & Saunders, Pearson India (2009)	
List of Additional Reading Material / Reference Books		
	Elementary Practical Organic Chemistry: Small Scale Preparations Part 1, Arthur Vogel, Pearson 2010.	
	Elementary Practical Organic Chemistry : Qualitative Organic Analysis Part 2, Arthur Vogel, Pearson 2010.	
	Elementary Practical Organic Chemistry : Quantitative Organic Analysis Part 3, Arthur Vogel, Pearson 2010.	

SEMESTER II

	Course Code: CHT 3007	Course Title: Chemistry of Transition Metals	Credits = 4		
	Semester: II		Total contact hours: 60	L 3	T 1
Course Outcomes (students will be able to.....)					
1	Understand the characteristic electronic and magnetic properties of coordination compounds				
2	Correlate the observed properties with the underlying molecular geometry and interactions				
3	Evaluate the stability and reactivity of the coordination compounds				
4	Propose a plausible mechanistic pathway to explain the observed reactivity of coordination compounds				
List of Prerequisite Courses					
	Undergraduate Inorganic Chemistry course				
Course Contents (Topics and subtopics)					
					Reqd. hours
1	Chemistry of elements of first transition series: Characteristic properties of d-block elements, properties of the elements of first transition series, their binary compounds and complexes, illustrating relative stability of their oxidation states, coordination number and geometry				6
2	Coordination compounds: Werners coordination theory and its experiments verification, effective atomic number concept, chelates, nomenclature of coordination compounds, isomerism in coordination compounds, valence bond theory (VBT) of transition metal complexes				8
3	Electronic spectra of transition metal complexes: Types of electronic transition, selection rules for d-d transitions, spectroscopic ground states, spectrochemical series, Orgela and Tanabe-Sugano diagrams for transition metal complexes (d^1 - d^9 states), calculations of Dq, B and beta parameters, charge transfer spectra, discussion of the electronic spectrum of $[\text{Ti}(\text{H}_2\text{O})_6]^{3+}$ complex ion.				8
4	Magnetic properties of transition metal complexes: Types of magnetic behaviour, methods of determining magnetic susceptibility, spin only formulas, L-S coupling, correlation of u and u_{eff} values, orbital contribution to magnetic moments, application of magnetic moment data for 3d metal complexes, anomalous magnetic moments and magnetic exchange coupling and spin crossover.				8
5	Metal ligand bonding in transition metal complexes: Limitations of VBT, an elementary idea of crystal field theory (CFT), crystal field splitting in octahedral, tetrahedral and square planar complexes, factors affecting crystal field parameters, limitations of CFT, Molecular Orbital Theory: Octahedral, tetrahedral and square planar complexes, pi-bond and MOT.				6
6	Thermodynamic and kinetic aspects of metal complexes: A brief outline of thermodynamic stability of metal complexes and factors affecting the stability. Substitution reactions of square planar complexes.				6
7	Metal ligand equilibria in solutions: Stepwise and overall formation constants and their interaction, trends in stepwise constants, factors affecting stability of metal complexes with reference to the nature of metal ion and ligand chelate effect and its thermodynamic origin, determination of binary formation constants by pH metry and spectrophotometry.				8
8	Reaction mechanism of transition metal complexes: Energy profile of a reaction, reactivity of metal complexes, inert and labile complexes, kinetic application of VBT and CFT. Kinetics of octahedral substitution, acid hydrolysis, factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism, substitution reactions in square planar complexes, the trans effect. Mechanism of substitution reaction, redox reactions, electron transfer reactions, mechanisms of				10

one electron transfer reactions, outer sphere type reactions, cross reactions, inner sphere type reactions.	
Reaction mechanism of racemization and isomerization reactions	
List of Text Books	
Concise inorganic Chemistry, J.D. Lee, Wiley India	
Inorganic Chemistry, P.W. Atkins	
Advanced Inorganic Chemistry, Cotton and Wilkinson	
List of Additional Reading Material / Reference Books	
Inorganic Chemistry: Principles of structure and reactivity: J. E. Huheey, E. A. Keiter, R. L. Keiter : Benjamin Cummings	

Course Code: CHT 3009	Course Title: Molecular Thermodynamics	Credits = 4		
		L	T	P
Semester: II	Total contact hours: 60	3	1	0
Course Outcomes (students will be able to.....)				
1	Outline the scope and importance of the three laws of thermodynamics			
2	Explain the origin of the macroscopic thermodynamic phenomena on the basis of molecular properties			
3	Establish a quantitative correlation between the macroscopic observable and microscopic properties			
4	Determine an appropriate model for representing the system and calculating the parameters			
List of Prerequisite Courses				
	Undergraduate Physical Chemistry course			
Course Contents (Topics and subtopics)				Reqd. hours
1	Revisiting the fundamental concepts – Laws of thermodynamics, Clausius inequality, Helmholtz and Gibbs free energy, Spontaneity, Maxwell's relations			4
2	Concept of probability, probability distribution functions, average values, standard deviations,			4
3	Boltzmann distribution law and its application, partition functions for distinguishable and indistinguishable particles, thermodynamic properties from partition functions			6
4	Molecular partition function, equipartition function			6
5	Properties of ideal gases from partition functions – pressure, entropy, free energy			8
6	Partition functions for chemical reactions, calculation of equilibrium constants			8
7	Multicomponent system – free energy and entropy of mixing, partial molar quantities and chemical potential, Models for solutions, ideal and real solutions, activity and activity coefficients, statistical model for solvation			4
8	Theories of specific heats of solids			4
9	Phase equilibria – lattice model for condensed phases, Gibbs Phase rule, Clausius-Clapeyron equation, stability of phases, thermodynamic description of phase			5

	transitions, lambda transitions- first order and second order phase transitions	
10	Electrochemical equilibria – Electrochemical potentials, Poisson-Boltzmann model for distribution of electrolytes, Debye-Huckel theory Solvent interactions, heats of hydration, hydration number, pair formation, Bjerrum theory	5
11	Determination of dissociation constants of weak acids, solubility product, stability constant and formula of a complex, liquid junction potential, mean ionic coefficient by EMF measurements	6
List of Text Books		
	Elements of Statistical Thermodynamics- L.K.Nash, Addison Wesley	
	Statistical Thermodynamics – B.J.McCelland, Chapman Hall	
List of Additional Reading Material / Reference Books		
	Physical Chemistry, P.W. Atkins	
	Thermodynamics and Statistical Thermodynamics – F.W.Sears, G.L.Salinger, Narosa	

	Course Code: CHT 3033	Course Title: Stereochemistry and Spectroscopy of Organic Compounds	Credits = 4		
	Semester: II	Total contact hours: 60	L	T	P
			3	1	0
Course Outcomes (students will be able to.....)					
1	Determine the stereochemistry of the organic compound and assign the related notations				
2	Predict the stable stereoisomers on the basis of thermodynamic / kinetic parameters				
3	Justify the observed stereochemical pathway for product formation in given reaction based on mechanistic details				
4	Understand the structural details using spectroscopic data for a compound				
5	Utilize spectroscopic tools as probe for elucidating the mechanistic and stereochemical details				
List of Prerequisite Courses					
	Undergraduate Organic Chemistry, Organic Reaction Mechanism				
Course Contents (Topics and subtopics)					Reqd. hours
1	Stereochemistry of – (i) compounds with two or more stereocentres. (ii) 3,4,5 membered ring compounds (iii) 6- membered ring compounds, mono and di substituted cyclohexanes (iv) fused ring compounds – decalins. (v) molecules with tricoordinate and tetracoordinate centres – N, S, Si, P, As. (vi) allenes, spiranes, biphenyls, ansa compounds, paracyclophanes, alkylidene cycloalkanes				6
2	Strain and strain energy , polycyclic compounds				2
3	Resolution methods: Types of racemic mixtures, resolution of racemic mixtures				2
4	Conformational analysis: Acyclic and cyclic compounds. Decalin				2
5	Topocity and prostereoisomerism: Homotopic ligands and faces, enantiotopic ligands and faces, diastereotopic ligands and faces.				2
6	Stereoselective synthesis: Additions, elimination, dihydroxylation, addition to carbonyl group – Felkin-Anh model,				6
7	Chiral synthesis: Different approaches. Chiral reagents and Chiral auxiliaries. Diastereoselective synthesis of alkenes, stereoselective alkylation of enolates.				6

	Asymmetric reactions: aldol reaction, Michael reaction, Sharpless epoxidation & dihydroxylation, oxidations and reductions aminohydroxylation; Katsuki-Jacobsen's catalyst-epoxidation, Hydrogenation, Diels-Alder reaction. Chiral borane reagents. Evan's aldol Salen Chemistry-catalysis, Kinetic resolution.	
8	Electronic transitions, Chromophores, Auxochromes, Bathochromic and hypsochromic shifts, Solvent effects, Measurement of transmittance and absorbance, Beer Lambert's Law.	2
9	Double beam UV spectrophotometer, Woodward – Fieser Rules for dienes, enones and aromatic compounds, Application of absorption measurement to qualitative analysis and quantitative analysis, Photometric titrations, Analysis of binary mixtures.	2
10	Vibrational Spectroscopy: Vibrational transitions, Selection rule, Modes of stretching and bending, FT-IR spectrophotometer.	2
11	Group frequencies, Factors affecting IR group frequency, NIR spectroscopy, Applications of vibrational spectroscopy in structural elucidation of organic compounds.	4
12	¹H NMR Spectroscopy: Recapitulation of basic principle, Nuclear spin states and magnetic moments, Chemical shifts, Factors affecting the chemical shift, Shielding mechanism and anisotropic effects.	6
13	Chemical exchange, Spin-spin splitting and its origin, Magnitude of coupling constant: One bond coupling, geminal, vicinal and long-range couplings, Magnetic equivalence, Karplus equation	4
14	Nuclear Overhauser effect, Pulse technique, Solid state NMR, Interpretation of spectra and simplification of complex spectra.	4
15	¹³C NMR Spectroscopy: Elementary idea, Chemical shift, Calculation of approximate chemical shift values, Coupling constants, Interpretation of simple CMR spectra, Proton coupled and decoupled ¹³ C NMR spectra, Off-resonance decoupling, DEPT spectrum and Structural applications in ¹³ C NMR.	4
16	Mass Spectrometry: Introduction, Ion production, Fragmentation, Stevenson's rule, Radical site and Charge site-initiated cleavage, Rearrangements, Cleavage associated with common functional groups, Molecular ion peak, Metastable ion peak, Nitrogen rule, LRMS and HRMS, Isotopic abundance and Interpretation of mass spectra.	6
List of Text Books		
	Stereochemistry of organic compounds: Ernest L. Eliel, Samuel H. Wilen : A Wiley-interscience Publication	
	Stereochemistry, conformation and mechanism, P.S. Kalsi, New Age International, 2005	
	Introduction to Spectroscopy, D.L. Pavia, G.M. Lampman, G.S. Kriz, J.R. Vyvyan, Cengage Learning India Pvt Ltd	
	Spectrometric Identification of Organic Compounds, Robert M. Silverstein, Francis X. Webster, Wiley	
List of Additional Reading Material / Reference Books		
	Stereochemistry of Organic compounds- Principles and Applications, D. Nasipuri, New Age International	
	Stereochemistry of Carbon compounds, E.L. Eliel, Tata-MacGraw Hill Education.	
	Basic Concepts in Organic Stereochemistry, Sunil Kumar Talapatra, Bani Talapatra, Springer Cham, January 2023	
	Organic Spectroscopy: William Kemp, Palgrave	
	Principles of NMR in one and Two Dimensions: R.R. Ernst, G. Bodenhausen, A. Wokaun: Oxford Science Publication	

Elective Paper II CHT XXXX

Practicals:

	Course Code: CHP 3008	Course Title: Inorganic / Instrumental Chemistry Laboratory	Credits = 2		
	Semester: II	Total contact hours: 60	L	T	P
			0	0	4
Course Outcomes (students will be able to.....)					
1	Synthesize and isolate the inorganic complexes from single step and two step procedures				
2	Characterize the synthesized complexes using appropriate analytical techniques				
3	Utilize the synthesized complexes for specific complexes for various applications				
4	Formulate the optimum synthesis and characterization protocol for the various complexes				
5					
List of Prerequisite Courses					
	Chemistry of Transition Metals, Instrumental Methods of Analysis				
Course Contents (Topics and subtopics)					Reqd. hours
1	Preparation and characterization of inorganic complexes containing Fe, Co, Ni, Cu, Zn, with N, and P containing ligands. Applications of these complexes for Organic coupling reactions like Heck, Suzuki, Stille and Sonogashira reactions.				35
2	Characterization of the catalysts and the products using various analytical techniques like UV-visible spectroscopy, IR spectroscopy, NMR spectroscopy, CHN analysis, gas chromatography, GC-MS, etc				25

CHP 3009 Field Project / Internship

4 week full-time internship or field project.

Semester III

	Course Code: CHT 3003	Course Title: Heterocyclic Chemistry	Credits = 4		
	Semester: III		Total contact hours: 60	L	T
			3	1	0
Course Outcomes (students will be able to.....)					
1	List the synthetic methodologies for various heterocyclic compounds				
2	Classify the heterocyclic compounds based on the physicochemical properties				
3	Select appropriate heterocyclic compounds for specific applications based on the properties				
4	Explain the stability and reactivity of heterocycles based on the structural features				
List of Prerequisite Courses					
	Organic Reaction Mechanisms, Undergraduate Organic Chemistry				
	Course Contents (Topics and subtopics)				
			Reqd. hours		
1	Introduction to heterocyclic chemistry, occurrence in nature and daily life applications such as drugs, dyes, optical brighteners, natural products.				4
2	Nomenclature: Nomenclature of heterocyclic compounds. Trivial, Hantzsch-Widman..				6
3	Polarity, tautomerism, aromaticity, basicity, electrophilic substitution				6
4	Small rings (three and four membered): aziridines, thiirane, azetidine, oxetane, thietanes properties. Ring strain in small rings: Baeyer strain, Pitzer strain				6
5	Reactions of small rings: JCC reagent, Jacobsen epoxidation, Paterno-Buchi reaction				6
6	Five membered: Thiophene, Furan, Pyrrole, Oxazoles, Thiazoles. Properties and reactivity				4
7	Retrosynthesis of heterocyclic compounds & synthesis of five membered heterocycles: Paal-Knorr, Knorr synthesis, Hantzsch synthesis				6
8	Six membered: Pyridine and related heterocycles. Properties and reactivity/aromaticity-Chichibabin reaction, electrophilic and radical mechanism for bromination				6
9	Six membered: Synthesis via Chichibabin reaction, Hantzsch synthesis, Bohlmann-Ratz, Conrad Limpach, other cyclization processes				6
10	Seven membered and fused ring systems: Diazepines, benzofurans, indole, benzopyrans, quinoline. Properties and synthesis				6
11	Heterocyclic natural products `synthesis: Nifedipine, Ciprofloxacin				4
List of Text Books					
	Heterocyclic Chemistry, J. A. Joules & K. Mills, Wiley-Blackwell publishing, 5 th Edition				
	The Chemistry of Heterocycles: Structures, Reactions, Syntheses and Applications, Wiley-VCH, 2 nd Edition				
List of Additional Reading Material / Reference Books					
	Heterocyclic Chemistry-II, R. R. Gupta, M.Kumar, V. Gupta, Springer (India)				

	Course Code: CHT 3006	Course Title: Quantum Chemistry	Credits = 4		
	Semester: III		Total contact hours: 60	L	T
			3	1	0
Course Outcomes (students will be able to.....)					
1	Understand the fundamental concepts of quantum mechanics in relation to atomic properties				
2	Apply the quantum chemical principles to simple molecules				
3	Select the appropriate approximations required to extend the application to larger / complex molecules				
4	Correlate the results from quantum chemical calculations with bulk properties of materials				
List of Prerequisite Courses					
	Basic Calculus and Matrix maths (Std XII), Undergraduate Physical Chemistry				
	Course Contents (Topics and subtopics)				Reqd. hours
1	Mathematical review: Matrices and determinants, polar, Cartesian and spherical coordinates, Legendre and Laugurre polynomials, Taylor and McLaurin series, linear and Hermitian operators				6
2	Historical background of quantum mechanics- failure of classical theory, wave particle duality, uncertainty principle, Postulates of Quantum mechanics, probabilistic interpretation of wave function, Schrodinger wave equation, Eigen values and operators. expectation values, Bohr correspondence principle				8
3	Applications of Schrodinger equation to simple systems – particle in a box, harmonic oscillator, rigid rotor				6
4	H and H like atoms- two particle problem, Schrodinger equation in spherical coordinates, representation of orbitals, radial and angular plots, probability functions				8
5	Approximation methods- variation and perturbation theorems				6
6	Multi electron systems- Electron spin- spin orbitals, Pauli principle, (Helium atom as example), Hartree product, Slater determinant, Hartree Fock methods, self-consistent field theory Slater type orbitals, coulomb and exchange operators, orbital energies and Koopman theorem				12
7	Chemical bonding in diatomic molecules- Born-Oppenheimer approximation, LCAO and MO theory- H^+ in ground electronic ₂ state and excited states, MO treatment of H_2 - Hietler- London treatment, singlet and triplet states, applications to homo and hetero nuclear diatomic molecules, VB theory and its treatment to H_2 .				8
8	Chemical bonding in polyatomic molecules- semi empirical method-Huckel theory, application to simple pi systems, An introduction to <i>ab initio</i> , DFT and MM methods				6
List of Text Books					
	Quantum Chemistry, I.N. Levine, fifth edition - Prentice Hall				
	Quantum Chemistry, J.P.Low, K.A. Peterson, 3 rd Edn., Elsevier				
	Quantum Chemistry, D. A. McQuarrie, Viva Books, New Delhi (2003)				
	Physical Chemistry, P. W. Atkins, Sixth Edition, Oxford University Press, Oxford				
	Physical Chemistry, G. M. Barrow, Fifth Edition, Tata McGraw Hill, New Delhi				
List of Additional Reading Material / Reference Books					
	Fundamentals of quantum chemistry- James E House- (second edition) – Elsevier academic Press				
	Modern quantum chemistry- Attila Szabo and Neil S Ostlund- Dover publications				
	Molecular Quantum Mechanics, Atkins and Friedman. Valence- C.A. Coulson, ELBS.				
	Introduction to quantum mechanics- L.Pauling and E.B.Wilson Quantum Chemistry, Ira N. Levine				

	Course Code: CHT 3011	Course Title: Organic Synthesis	Credits = 4		
	Semester: III	Total contact hours: 60	L	T	P
			3	1	0
Course Outcomes (students will be able to.....)					
1	Understand the disconnection and retrosynthetic approach for organic molecules				
2	Select the appropriate synthetic approach for introducing functional group or structural features				
3	Select the optimum reagents for the oxidation / reduction of molecular groups towards synthesizing the final product				
4	Choose the suitable name reactions for the given retrosynthetic protocol				
List of Prerequisite Courses					
	Undergraduate Organic Chemistry, Organic Reaction Mechanism, Stereochemistry and Spectroscopy of Organic Compounds				
Course Contents (Topics and subtopics)					
					Reqd. hours
1	Disconnection approach and retrosynthetic analysis. Planning of multistep synthesis. Concepts of synthons, retrons and synthetic equivalents. Generation of structural complexity using tandem and cascade processes. Concepts in organic synthesis: linear and convergent synthesis, Umpolung concept, umpolung of reactivity and protecting groups.				7
2	Functional groups: Their reactivity profile, interconversions and protection.				4
3	Ylides: Ylides of P, N and S. Wittig reaction and its modifications,				4
4	Enamines: Synthesis, reactivity and synthetic importance.				2
5	Ring synthesis/cyclization methods: Baldwin Rules, some important Stereoelectronic effects relevant to Organic Synthesis. Different approaches towards the synthesis of three, four, five, and six-membered rings, Bergman cyclization; Nazarov cyclization, cation-olefin cyclization and radical-olefin cyclization, inter-conversion of ring systems (contraction and expansion). Construction of macrocyclic rings				4
6	Reduction: Catalytic hydrogenation. Dissolving metal reductions. Hydride transfer reagents. Complex hydrides including nucleophilic, electrophilic and radical reducing agents. Organo boranes. MVP reduction.				6
7	Oxidation: Cr, Os, Ti, Fe and Mn reagents, peracids and peroxides, Oxidation by ozone and oxygen, Swern oxidation. Baeyer-Viliger oxidation.				6
8	Selected organic reagents: TMSCl, TBTH, DCC, DDQ, TCQ, CAN, NBS, DIBAL, PTC, Crown ethers, Sml ₂ , SeO ₂ Corey-Chaykowsky reagent, DABCO, Gilman's reagent, Lawesson reagent, Simmon-Smith reagent.				6
9	Selected name reactions: Wittig reaction, Shapiro reaction, Paterson olefination, Birch reduction, Woodward-Prevost reaction, Mukaiyama esterification, Mitsunobu reaction. Finkelstein reaction, Buchwald-Hartwig amination, Baylis-Hilman reaction, Corey-Fuchs reaction, Ritter reaction, Bestman-Ohira reagent, Chemo, regio and stereoselective transformations. Barton deoxygenation and decarboxylation.				7
10	Rearrangements: Favorskii reaction, Curtius Lossen, Benzil-Benzilic acid rearrangement, Steven, Tiffenev-Demyanov, Benzidine rearrangement, Baker-Venkatraman rearrangement, Ireland-Claisen rearrangement, Wittig rearrangements. Common named reactions and rearrangements – applications in organic synthesis.				8
11	The Art of Organic Synthesis: snippets of some multistep syntheses, Natural products, the advent of ancillary methods, teaching new tricks to old dog strategies approach, etc				6

List of Text Books		
	Organic synthesis Michael B. Smith: McGraw-Hill	
	Modern Organic Synthesis: An Introduction By George S. Zweifel, Michael H. Nantz, Peter Somfai · 2017.	
	Strategic Applications of Named Reactions in Organic Synthesis, Laszlo Kurti, Barbara Czako · 2005	
	Organic Chemistry Clayden, Greeves, Warren and Wothers: Oxford University Press	
	Principles of Organic Synthesis, R.O.C. Norman; Blackie academic and Professional	
	Organic synthesis: The Disconnection Approach, S.G. Warren and P. Wyatt, John Wiley & Sons	
	Organic synthesis Michael B. Smith: McGraw-Hill	
List of Additional Reading Material / Reference Books		
	Modern Organic Synthesis: An Introduction By George S. Zweifel, Michael H. Nantz, Peter Somfai · 2017.	
	Strategic Applications of Named Reactions in Organic Synthesis, Laszlo Kurti, Barbara Czako · 2005	
	Organic Chemistry Clayden, Greeves, Warren and Wothers: Oxford University Press	
	Principles of Organic Synthesis, R.O.C. Norman; Blackie academic and Professional	
	Organic synthesis: The Disconnection Approach, S.G. Warren and P. Wyatt, John Wiley & Sons	

Elective Paper III CHT XXXX

Practicals:

	Course Code: CHP 3010	Course Title: Physical and Computational Laboratory	Credits = 4		
	Semester: III	Total contact hours: 60	L	T	P
			3	1	0
Course Outcomes (students will be able to.....)					
1	Determine the thermodynamic parameters of physical and chemical equilibria				
2	Analyze physicochemical data to derive important correlations between structure and solubility / reactivity / etc.				
3	Develop appropriate protocols to determine properties like isoelectric point, pKa with high accuracy and precision				
4	Evaluate different physicochemical methods based on the sensitivity and accuracy of measuring physical properties				
5					
List of Prerequisite Courses					
	Quantum Chemistry, Undergraduate Physical Chemistry course				
Course Contents (Topics and subtopics)					Reqd. hours
1	Molecular modeling: Introduction to Molecular modeling, Structure building, Optimization, Force fields and algorithms, Z-matrix, Hydrogen bonding, Intermolecular Hydrogen bonding, Applications in supramolecular assemblies Complexes and binding energies, Semi empirical (MOPAC) calculations Frequency analysis, HOMO-LUMO analysis, Analysis stationary states and				20

	Transition states, Ab initio and DFT calculations	
2	Learning Programming language – Python: Introduction to Python GUI, Arithmetic rules - Maths Module, Creating script file, Looping, Adding counter to program if else and while, Boolean algebra, Creating own functions, import Generating and appending output files	20
3	Determination of thermodynamic parameters and partial molar volume Determination of iso electric points Experiments based on phase equilibrium Conductometric and potentiometric titrations of multi component systems Determination of solubility products, stability constants, thermodynamic data from measurements	20
List of Text Books		
	“Experiments in Physical Chemistry” by D.P. Shoemaker, C.W. Garland, and J.W. Nibler, McGraw-Hill	
	Practical Physical Chemistry. By Dr. A. Findlay. Third edition. London: Longmans, Green and Co., 1914.	

CHP 3011 Research Project – 1

Part 1 of the mandatory research project. Rules and regulations for the same to be decided by Head of the Department.

SEMESTER IV

	Course Code: CHT 3010	Course Title: Radicals, Photochemistry and Pericyclic Reactions	Credits = 4		
	Semester: IV		Total contact hours: 60	L	T
			3	1	0
Course Outcomes (students will be able to.....)					
1	Identify the important reactive intermediates and list their properties				
2	Discuss the various reaction mechanisms and the influence of various factors on the mechanism				
3	Estimate the plausible reaction mechanism and the experimental methods to verify the same				
4	Evaluate the mechanistic details involving different reactive intermediates based on properties of reacting molecules				
List of Prerequisite Courses					
	Organic Reaction Mechanism, Organic Synthesis				
Course Contents (Topics and subtopics)					
			Reqd. hours		
1	Radicals: Generation of radicals. Stability of radicals, Nucleophilic and electrophilic radicals. Characteristic reactions - Free radical substitution, addition to multiple bonds.				4
2	Radicals in synthesis: Inter and intra molecular C-C bond formation via mercuric hydride, tin hydride, thiol donors. Cleavage of C-X, C-Sn, C-Co, C-S, O-O bonds. Oxidative coupling. C-C bond formation in aromatics: S _N Ar reactions. Hoffman-Löffler-Freytag reaction.				10
	Photochemistry:				
3	Excited state: Jablonski diagram - Fluorescence, phosphorescence. Principle of energy transfer. Chemical reactivity of electronically excited molecules - orbital character, acidity, redox, etc. Exciplex formation. Triplet sensitization and delayed fluorescence				3
4	Photosensitized reactions, chemiluminescence. Photosensitization, quenching, quantum efficiency, and quantum yield				3
5	Photochemical reactions: Substitution, oxidation, reduction. photoreactions: Isomerism, Paterno-Buchi, Norrish reactions, Photoreduction of ketones, Photochemistry of arenes, Barton, Di-pi methane rearrangement. Photochemistry of - olefins, dienes, carbonyl compounds, arenes. PhotoFries reaction, Barton reaction. Synthesis of Cubane, adamantane, etc. Flash photolysis and lasers				10
	Pericyclic Reactions:				
6	Recapitulation of molecular orbitals and their symmetry properties. Classification of pericyclic reactions, Thermal and photochemical transformations				4
7	Electrocyclic reactions: 4n and 4n+2 electron systems, FMO theory, Conservation of orbital symmetry, Woodward Hoffmann rule and Huckel Mobius approach				10
8	Cycloaddition reactions: Principles and its application in chemical reactions. FMO theory, Conservation of orbital symmetry, Woodward Hoffmann rule and Huckel Mobius approach, Endo rule, Cheletropic reactions, 1,3- dipolar reactions				10
9	Sigmatropic rearrangements: [i,j] shifts, FMO approach, Cope and Claisen rearrangements, Group transfer reactions: Ene reaction				6
List of Text Books					
	Frontier Orbitals and organic Chemical reaction: Ian Fleming				
	Organic photochemistry, Coxon, Oxford University Press				

List of Additional Reading Material / Reference Books	
Advanced Organic Chemistry: Part A and B: Francis Carey	
Introduction to Organic photochemistry, J.D. Coyle, Wiley	

Course Code: CHT 3015	Course Title: Solid state Chemistry and Group Theory	Credits = 4		
		L	T	P
Semester: IV	Total contact hours: 60	3	1	0

Course Outcomes (students will be able to.....)

1	Define the various packing arrangements in solids	
2	Classify the given solid on the basis of the crystal lattice and associated parameters	
3	Understand the correlation between the structural features and solid state packing in solids	
4	Apply principles of group theory to explain symmetry and resulting applications	

List of Prerequisite Courses

Molecular Thermodynamics, Matrix algebra (Std XII)	
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Course Contents (Topics and subtopics)

		Reqd. hours
1	Solid state chemistry	
	1.1 An introduction to crystal structure- lattice types and unit cells, Miller indices, close packing	4
	1.2 Synthesis of solid state materials- ceramic, co precipitation, sol gel methods, micro wave and combustion synthesis, hydro thermal methods, kinetics of solid state reactions	6
	1.3 Characterization of solids- diffraction methods- X ray, electron and neutron diffraction, electron microscopy, EDAX, XANES techniques	6
	1.4 Bonding in solids- Ionic crystals, lattice energy of ionic crystals, metallic crystals. Band theory and electronic conductivity, Zone theory- Brillouin zones, k – space, Fermi surfaces and density states	4
	1.5 Properties of solids- metals, semiconductors and p-n junctions, super conductors- theory and applications, ionic conductivity, photo conductivity, defects in solids, non-stoichiometry Optical properties- lasers, light emitting diodes Magnetic and dielectric properties- types of magnetic properties, magnetic resistance	10
2	Molecular symmetry and Group theory	
	2.1 Introduction to molecular symmetry – symmetry elements and operations.	4
	2.2 Classification and assignment of point groups to Inorganic molecules, multiplication tables and matrix representation – unitary and reducible representations	6
	2.3 The great orthogonality theorem, character tables	6
	2.4 Applications of group theory to chemical bonding (hybrid orbitals for σ -bonding in different geometries and hybrid orbitals for π -bonding. Symmetries of molecular orbitals.	8
	2.5 Application of Group Theory to vibrational spectroscopy: A brief idea about Infrared and Raman scattering spectroscopy, vibrational modes as basis of group representations	6

10		
List of Text Books		
	Solid state Chemistry- An Introduction - Lesley E Smart and Elaine A Moore – Third edition, Taylor and Francis.	
	F. A. Cotton, Chemical applications of Group theory, Third Edition, John Wiley & Sons, New York, 1990.	
	D. M. Bishop, Group Theory and Chemistry, Dover Publications, New York, 1977	
	Solid State Chemistry and its Applications, 2nd Edition, Student Edition Anthony R. West, Wiley	
List of Additional Reading Material / Reference Books		

	Course Code: CHT 3034	Course Title: Organometallic Chemistry and Catalysis	Credits = 4		
	Semester: IV	Total contact hours: 60	L	T	P
			3	1	0
Course Outcomes (students will be able to.....)					
1	Understand the basic properties for organometallic compounds				
2	Explain the observed properties on the basis of structure and bonding in organometallics				
3	Select the suitable organometallic compounds for applications as catalysts in organic transformations				
4	Develop synthesis and characterization protocols for organometallics based on the desired structure and applications				
List of Prerequisite Courses					
	Organic Synthesis, Chemistry of Transition Metals				
	Course Contents (Topics and subtopics)				
	Reqd. hours				
1	History of Organometallic Chemistry: Nobel prizes awarded to this field and applications				
2	Basic concept: Werner complexes, trans effect, Soft versus Hard ligands, Back bonding, Electroneutrality, Types of ligand				
3	General Properties of Organometallic Complexes: 18- electron rule and its limitation, Electron counting in reactions, Bridged complexes, Metal-metal bond. Associative-Dissociative mechanisms				
4	Classification of reactions: Oxidative addition, reductive elimination, insertion, β -Hydride elimination, σ -Bond metathesis, π -Bond metathesis				
5	Complexes of π -Bound Ligands: Backbonding concept for explaining metal-alkene and alkyne interactions. Alkene and Alkyne complexes allyl complexes, Diene complexes, Cyclopentadienyl complexes, Arenes and other alicyclic ligands.				
6	Reactions of Metal-alkyls, metal-alkenes and metal-alkynes: Tsuji-Trost allylic alkylation, Reppe reaction, Pauson and Khand reaction				
7	Carbonyls Complexes: Backbonding concept for explaining metal-carbonyl interactions. Metal complexes of CO ligands, Dissociative substitution, Associative mechanism. Substitution reactions of Metal-CO complexes				
8	Phosphine complexes: Bonding concept for explaining metal-phosphine interactions. Substitution reactions and the effect variation in electronic properties of phosphine on reactivity. Tolman's Cone angle concept				
8	Bio-organometallic Chemistry: Basic concept of metals in biology having metal-				

	carbon bond, cyanocobalamin, carboxyhaemoglobin, carbon monoxide dehydrogenase	
9	Metal–Ligand Multiple Bonds: Carbenes, Carbynes, Bridging Carbenes and Carbynes, N-Heterocyclic carbenes, Multiple bonds to heteroatoms, Applications of organometallic chemistry, Alkene metathesis; Dimerization, oligomerization, and polymerization of alkenes, Activation of CO and CO ₂ , CH.	3
10	Organometallic chemistry for meeting future challenges: Environment remediation for CO ₂ utilization and depolymerization	2
11	Physical Methods in Organometallic Chemistry: Isolation procedures, ¹ H, ¹³ C and ³¹ P NMR, Dynamic NMR, Spin saturation transfer, IR Spectroscopy, Crystallography, Other methods	4
12	Types of catalysis: Heterogeneous and Homogeneous catalysis. Catalytic cycles. TON, TOF	2
13	Catalyst preparation: Bulk and supported catalysts, deactivation and regeneration.	3
14	Characterization of catalysts: Surface area, surface acidity and basicity, XPS, UPS, AES, EXAFS, XANES, XRD TPD.	6
15	Heterogeneous catalysis: Adsorption isotherms, kinetics of heterogeneous catalytic reactions, structure of adsorbed species.	3
16	Catalysis using solid acids and bases: Zeolites, mesoporous materials and clays as catalysts, shape selectivity. Catalysis by metals, metal oxides. Application in bulk chemicals, environment, energy, photocatalysis. catalyst deactivation.	3
17	Homogeneous Catalysis: Applications in reactions - hydrogenation (Wilkinson catalysts), carbonylation, hydroformylation, Hydrocyanation of butadiene, coupling reactions - Suzuki coupling, Heck coupling and related cross coupling reactions. Alkene oligomerization and metathesis. Ziegler-Natta catalysts, Alkene hydrosilation and hydroboration,	8
18	Catalytic oxidations and reductions, epoxidation, dihydroxylations, decarbonylation, olefin isomerization, arylation, polymerization, asymmetric synthesis, heterogenised homogeneous catalysts, phase transfer catalysis, catalysis in green chemistry, Chiral ligands and chiral induction	6
List of Text Books		
	The organometallic chemistry of the transition metals, Robert H. Crabtree, John Wiley & Sons	
	Organometallic Chemistry of Transition elements: F. P. Pruchnik: Springer	
	Organometallic Chemistry : R. C. Mehrotra: New Age International	
	Organometallic Chemistry: G. S. Sodhi: Ane Books Pvt. Ltd.	
	Organometallic reagents in Organic Synthesis: Paul R. Jenkins: Oxford Science Publications	
	Catalysis from principles to applications, Eds. Matthias Beller, Albert Renken and Rutger A. van Santen, Wiley-VCH	
	Principles and practice of heterogeneous catalysis -	
List of Additional Reading Material / Reference Books		
	Catalysis- concepts and green applications- Gadi Rothenberg-Wiley VCH	
	Homogeneous	
	Design of heterogeneous catalysts –U.S.Ozkan (ed) – Wiley VCH	
	Introduction to surface chemistry and catalysis- G.A. Somarjai, Wiley and sons.	
	Heterogeneous catalysis, D.K. Chakrabarty and B. Viswanathan, New Age Publishers, New Delhi	

Elective Paper IV CHT XXXX

CHP 3012 Research Project – 2

For the project guides will be allotted by the Head. The guide will assign research topics to the students. The students are expected to work under the supervision of the guides. At the end of semester IV thesis will be submitted as the prescribed schedule. The thesis will be evaluated by the guide and one external examiner and viva voce will be conducted.

ELECTIVE PAPERS

	Course Code: CHT 3013	Course Title: Industrial Chemistry	Credits = 4		
	Semester: XX	Total contact hours: 60	L	T	P
			3	0	1
Course Outcomes (students will be able to.....)					
1	Recall the principles for manufacture of bulk chemicals				
2	Explain the synthetic approaches for obtaining the primary inorganic compounds				
3	List the various organic chemicals manufactured and the standard process used for the same				
4	Suggest or design improvements for the current processes to address concerns				
List of Prerequisite Courses					
	Organic Synthesis, Organometallic Synthesis and Catalysis				
Course Contents (Topics and subtopics)					
			Reqd. hours		
1	Types of Chemicals. Status of global and Indian Chemical Industry				2
2	Operation and Processes in Petrochemical Industry				4
3	Physicochemical principles of manufacture of important organic bulk chemicals such as methanol, acetic acid, ethanol, ethylene, propylene, butadiene, acetaldehyde, acetylene, BTX, alkyl benzenes, acetone, phenol, styrene, esters, ethylene oxide, phthalic acid, Vinyl-Halogen and Vinyl-Oxygen Compounds, azo dyes, Polyamides, Propene Conversion Products, Aromatics - Production and Oxidation Products of Xylene and Naphthalene, important pharmaceutically active ingredients, agrochemicals, insecticides, pesticides etc				20
4	PRIMARY INORGANIC MATERIALS: Water, Hydrogen, Hydrogen Peroxide and Inorganic Peroxo Compounds, Nitrogen and Nitrogen Compounds, Phosphorus and its Compounds, Sulfur and Sulfur Compounds, Halogens and Halogen Compounds, MINERAL FERTILIZERS: Phosphorus-Containing Fertilizers, Nitrogen-Containing Fertilizers, Potassium-Containing Fertilizers				12
5	METALS AND THEIR COMPOUNDS: Alkali and Alkaline Earth Metals and their Compounds Aluminum and its Compounds, Chromium Compounds and Chromium, Silicon and its Inorganic Compounds, Manganese Compounds and Manganese				6
6	ORGANO-SILICON COMPOUNDS: Industrially Important Organo-Silicon Compounds Industrially Important Silanes, Silicones, Industrial Silicone Products INORGANIC SOLIDS: Silicate Products, Inorganic Fibers, Construction Materials, Enamel Ceramics, Metallic Hard Materials, Carbon Modifications, Fillers, Inorganic Pigments				10
7	NUCLEAR FUEL CYCLE: Economic Importance of Nuclear Energy, General Information about the Nuclear Fuel Cycle, Availability of Uranium, Nuclear Reactor Types, Nuclear Fuel Production Disposal of Waste from Nuclear Power Stations				6
List of Text Books					
	Industrial Organic Chemistry, 3rd, Completely Revised Edition, Klaus Weissermel, Hans-Jürgen Arpe ISBN: 978-3-527-61459-2 July 2008				
	Industrial Inorganic Chemistry, 2nd Completely Revised Edition, Karl Heinz Buchel, Hans-Heinrich Moretto, Dietmar Werner, ISBN: 978-3-527-61333-5, 667 pages, November 2008, Wiley-VCH.				

	Course Code: CHT 3016	Course Title: Biochemistry	Credits = 4		
	Semester: XX	Total contact hours: 60	L	T	P
			3	0	1
Course Outcomes (students will be able to.....)					
1	List the various properties and functional importance of different class of biomolecules				
2	Explain the reactivity and functions of enzymes based on the concept of active sites				
3	Understand the biogenesis pathways for the important classes of biomolecules				
4	Apply the bioenergetic principles to explain the functional features of biomolecules				
List of Prerequisite Courses					
	Undergraduate Organic Chemistry course, Undergraduate Physical Chemistry course				
Course Contents (Topics and subtopics)					
					Reqd. hours
1	Proteins: Purification and characterization. Amino acid sequence, method of determining the sequence - Use of MALDI. Peptide synthesis. Biologically active peptides. Protein conformation and biological functions.				8
2	Nucleic acids: Conformation and function of DNA and RNA, genetic code, mutation, recombinant DNA, DNA synthesis, DNA biosynthesis and related drugs.				10
3	Enzymes: Nomenclature, classification, isolation, concept of active site, affinity labeling and enzyme modification, Microbial reactions, enzymes in organic solvent, enzyme mechanisms, Enzyme inhibitors. Enzyme specificity (region-, stereo-, functional), chymotrypsin, Nuclease (endo and exo), lysozyme and carboxypeptidase A, cytochrome 450, cofactors as derived from vitamins, coenzymes, prosthetic groups, apoenzymes.				12
4	Structure and biological functions of - coenzyme A, thiamine pyrophosphate, pyridoxyl phosphate, NAD ⁺ , NADP ⁺ , FAD, FMN, flavin dinucleotide, vit B12.				8
5	Bioenergetics: Standard free energy change in biological systems, hydrolysis of ATP, ADP → ATP, Glucose storage, metal complexes in transmission of energy; chlorophylls, Photosystem I and photosystem II in cleavage of water. Enzyme kinetics. MM equation.				8
6	Biogenesis and biosynthesis of natural products: Concept of biological chemistry. Primary and secondary metabolites, methods used in study of biosynthesis. Polyketide and Shikimic acid pathway, polyketides, terpenes and steroids.				8
7	Carbohydrates and Lipids: Structure, classification, characterization, metabolism				6
List of Text Books					
	Biotransformations in Organic Chemistry: Kurt Faber: Springer				
	Principles of Biochemistry, Lehninger, 4 th Edition				
	Biochemistry, Voet and Voet, 3 rd Edition.				
	Biochemistry, Garret and Griesham				
	Bioorganic Chemistry, Dugas, H, Springer				
List of Additional Reading Material / Reference Books					
	Bioorganic Chemistry – Carbohydrates and Nucleic acids, Hecht (editor)				
	Bioorganic Chemistry, Soni, R.K. and Sharma, P, Saujanya Book, 2008				

	Course Code: CHT 3018	Course Title: Chemistry of Main Group Elements	Credits = 4		
	Semester: XX	Total contact hours: 60	L	T	P
			3	0	1
Course Outcomes (students will be able to.....)					
1	Understand the correlation between the properties and structural features of main group elements				
2	Enlist the important properties of the various compounds of main group elements				
3	Examine the electronic structure and properties of lanthanides and actinides				
4	Explain the bonding and applications for metal clusters based on the structure				
List of Prerequisite Courses					
	Undergraduate Inorganic Chemistry course				
	Course Contents (Topics and subtopics)				
					Reqd. hours
1	Periodic table, periodic trends in atomic properties Reactivity of chemical species including Latimer diagram: Construction of the diagram, non-adjacent species and disproportionation. Frost Diagram: Construction and interpretation. Pourbaix diagram of Iron in natural water				4
2	s-block elements: Salient features of hydrides, solvation and complexation tendencies, function in biosynthesis.				8
3	p-block elements: Hydrides, oxides, oxyacids, and halides, hydrides of boron - diborane and higher boranes, borazine, borohydrides, fullerenes, carbides tetrasulfur tenitride.				10
4	Streochemistry and bonding in main group elements: VSEPR, Walsh diagrams (tri- and penta-atomic molecules), $d\pi$ - $p\pi$ bonds, Bent rule and energies of hybridization. Simple reactions of covalently bonded molecules.				8
5	Lanthanides: Occurrence and isolation, separation. Electronic structure, oxidation states. Lanthanide contraction and ionic radii. lanthanide compounds and complex formation.				6
6	Actinides: General features and chemistry of actinides, chemistry of separation of Np, Pu and Am from U. Similarities between				8
7	Silicones and Phosphazenes: Silicones and phosphazenes as examples of inorganic polymers, nature of bond in triphosphazines. Later actinides and later lanthanides.				8
8	Metal clusters: Higher boranes, carboranes, metalloboranes and metallocarboranes, metal carbonyls and halide clusters, compounds with metal-metal multiple bonds.				8
List of Text Books					
	J.D. Lee, <i>Concise Inorganic Chemistry</i> ; Wiley India				
	Inorganic Chemistry, P.W. Atkins				
	Advanced Inorganic Chemistry, Cotton and Wilkinson				
	Inorganic Chemistry: Principles of Structure and Reactivity: J. E. Huheey, E. A. Keiter, R. L. Keiter : Benjamin Cummings				

	Course Code: CHT 3021	Course Title: Natural Products	Credits = 4		
	Semester: XX	Total contact hours: 60	L	T	P
			3	0	1
Course Outcomes (students will be able to.....)					
1	Understand the structure, classification and role for important natural products				
2	List the synthetic pathways for the important natural products				
3	Determine the important structural features of natural products using suitable techniques and interpreting the data				
4	Modify the structural features of natural products for better compatibility with the desired applications				
List of Prerequisite Courses					
	Organic Synthesis, Biochemistry				
Course Contents (Topics and subtopics)					
			Reqd. hours		
1	General introduction about naturally occurring molecules and their importance.				4
2	Steroids: Occurrence, structure, classification, biological role, biosynthesis pathway. Nobel prizes related to steroids. Important structural and stereochemical features of cholesterol, ergosterols, bile acids, steroidal hormones.				6
3	Steroids: Synthesis of cholesterol, Taxol synthesis, progesterone synthesis, estrone synthesis				6
4	Terpene and terpenoids: Occurrence, structural importance, types of terpenoids. Isoprene rule and identification of isoprene units in naturally occurring molecules. Synthesis of (R)-Citronellol, Menthol, Ethyl farnesoate.				6
5	Carbohydrates: Anhydro-, amino-, branched chain, unsaturated sugars. Oligo and poly-saccharides. Sugars as raw materials. Configurational assignments of monosaccharides, Structure determination of disacchirides – lactose. Inositols. Constitution and application of chitin. Amylose and amylopectin, cellulose, hemicelluloses, glycogen, inulin, sulphated polysaccharides.				6
6	Nucleosides: DNA as a molecule of life. Evolutionary development, coding in protein synthesis, nucleosides, nucleotides, glycosidic bond with sugars, DNA structure.				4
7	Nucleoside based drugs, antivirals, anticancer, mode of action, fluorescent probes. Synthesis of FV-100, BVDU, Toyocamycin, Sangivamycin, Alogliptin				6
8	Plant pigments: General structural features, occurrence, isolation, biological importance, and applications of - carotenoids, anthocyanins, flavones. Structure determination and synthesis of B-carotene.				6
9	Prostaglandins: Classification and biological importance. Structure determination and synthesis of PGE1 and PGF1.				4
10	Insect pheromones: Structural features, classification, and importance. Synthesis of bombycol and gossyplure.				4
11	Plant growth regulators and insect growth regulators: genral idea, structure, examples and applications. Synthesis of pyrethrin, chrysanthemic acid, metofluthrin.				6
List of Text Books					
	Chemistry of Natural Product: Sujata V. Bhat, Bhimsen A. Nagasampagi, M. Sivakumar: Springer.				
	Terpenoids: V. K. Ahluwalia: Ane Books Pvt. Ltd.				
	Steroids and Hormones: V. K. Ahluwalia: Ane Books Pvt. Ltd.				
	Antibiotics : V. K. Ahluwalia: Ane Books Pvt. Ltd.				
List of Additional Reading Material / Reference Books					
	Organic Chemistry of Natural Products, G. R. Chatwal: Himalaya Publications, New Delhi				

	Course Code: CHT 3022	Course Title: Polymer Chemistry	Credits = 4		
	Semester: XX	Total contact hours: 60	L	T	P
			3	0	1
Course Outcomes (students will be able to.....)					
1	Understand the characteristic properties of polymers				
2	Outline the important strategies for synthesis of different types of polymers				
3	Analyze the characterization data of polymers to understand the macroscopic and molecular properties				
4	Select the appropriate polymers for a given application				
5					
List of Prerequisite Courses					
	Undergraduate Physical Chemistry, Organic Synthesis				
Course Contents (Topics and subtopics)					Reqd. hours
1	Monomers: Their sources and synthesis				4
2	Methods of polymerization: Bulk, Solution, Suspension, Emulsion, Addition, Melt, Condensation.				8
3	Mechanisms of polymerization: Ionic and coordination polymerization. Step-Grown vs chain growth. Degree of polymerization.				8
4	Properties of polymers: Viscosity, end-group analysis, hardness, abrasion resistance Structure and properties: Morphology and crystallinity, Molecular weight distribution- Number and weight average molecular weight. Polydispersity, crystallinity. Glassy state - Glass transition temperature Tm and Tg. Stereochemistry.				8
5	Additives in polymers: Plasticizers, stabilizers, antioxidants, fillers, pigments, etc.				8
6	Synthesis and properties of important polymers: PE, PVC, PVA, Polyacrylates, Polystyrene, Teflon, ABS, SBR, SAN, Nylons, polyesters, polyurethanes, polycarbonates, cellulose esters, cellulose nitrates. Thermosets: Phenol formaldehyde, urea formaldehyde, melamine formaldehydes, epoxy resins. Silicones living polymers, metathesis polymerization.				10
7	Processing of polymers: Compounding, calendaring, die/rotational/film casting, injection molding, extrusion molding, thermoforming, foaming, reinforcing				12
8	Advanced polymers				2
List of Text Books					
	Polymer Science: V. R. Gowariker, N.V.Vishwanathan, Jayadev Sreedhar New Age International (P) Limited, Publisher.				
	Polymers: David Walton and Phillip Lorimer: Oxford Science publications				
List of Additional Reading Material / Reference Books					
	Polymer Science: V. K. Ahluwalia, Anuradha Mishra: Ane Books pvt. Ltd.				

	Course Code: CHT 3023	Course Title: Surface and Interfacial Chemistry	Credits = 4		
	Semester: XX		Total contact hours: 60	L	T
			3	0	1
Course Outcomes (students will be able to.....)					
1	Understand the variation of structural features at the interface and the resulting effect on properties				
2	Utilize the information from various characterization techniques to understand interfacial features				
3	Explain the interfacial properties by applying various models to the interfacial systems				
4	Design surfactants / colloids for a given application using the various surface properties				
List of Prerequisite Courses					
	Molecular Thermodynamics				
Course Contents (Topics and subtopics)					
			Reqd. hours		
1	Concept of surface free energy and surface tension, interfacial tension and interfacial free energy, surface excess.				
2	Liquid surfaces				
	2.1 Thermodynamics of liquid surfaces: Gibbs adsorption isotherm, spreading coefficient and wetting phenomena.				
	2.2 Thermodynamics of curved surfaces: Young, Laplace, Kelvin, and Thomson equations.				
	2.4 Potentials of interfaces, interfacial viscosity. Insoluble monolayers, LB films and molecular self assembly.				
	2.4 Bubbles and foams, homogeneous and heterogeneous nucleation.				
3	Solid- liquid interfaces: Work of adhesion and cohesion, wetting and contact angles, adsorption from solution at solid/ liquid interfaces, critical surface tension.				
4	Surfactants				
	Introduction: General structure, types, nomenclature Surfactant aggregates – Factors affecting aggregational behaviour				
	Synthesis of surfactants: Synthesis of hydrophobes, functionalisation of hydrophobes				
	Applications of surfactants, Biosurfactants and biodegradable surfactants, Mixed surfactant systems				
5	Emulsions, microemulsions, gels, foams, colloids.				
6	Hydrotropes: Nature, structure, behavior, applications				
List of Text Books					
	An introduction to the principles of surface chemistry- Aveyard				
	Micelles- Theoretical and applied aspects- Y.Morai				
	Surface activity- principles and applications- Kaoru Tsujii				
	Fundamentals of colloid science- Robert J Hunter- Vol I and II				
	Colloid chemistry- Shaw				
	Surfaces, interfaces and colloids, Meyers				
List of Additional Reading Material / Reference Books					
	Physical Chemistry of surfaces, Adamson				
	Surfactant and Interfacial phenomena by M.J. Rosen, 2 nd Edition, Wiley Interscience publications 1989				
	Surfactants: Chemistry and properties by Anthony JO'Lenick Illinois: Allured publication 1999				

	Course Code: CHT 3024	Course Title: Computational Chemistry	Credits = 4		
	Semester: XX	Total contact hours: 60	L	T	P
			3	0	1
Course Outcomes (students will be able to.....)					
1	Demonstrate the use of computers for calculations of molecular properties of simple molecules				
2	Use the advanced semi-empirical methods for modelling the more complex molecules				
3	Explain the experimental observations of the molecular systems or processes using the computational results				
4	Use molecular dynamics techniques for modelling larger systems and elucidate their properties				
List of Prerequisite Courses					
	Quantum Chemistry				
Course Contents (Topics and subtopics)					Reqd. hours
1	Introduction to Computational Chemistry, Basic concepts				4
2	Molecular Mechanics methods, Optimization methods, Defining Geometry and Z-matrix				8
3	Electronic structure - methods: Schrodinger Equation, Born– Oppenheimer Approximations, SCF Theory, Energy of Slater Determinant, Koopmans' Theorem, Basis Set Approximation, Basis Sets				8
4	Hartree-Fock Approximation, Correlation, Moeller-Plesset Perturbation Theory, Configuration Interaction, Multi-configurational Self-consistent Field				8
5	Semiempirical Methods				10
6	Density Functional Theory				4
7	Applications in Drug Designing, Statistics and QSAR, Applications in Catalysis				6
8	Simulation Techniques: Monte Carlo Methods, Molecular Dynamics, Solvation Models, Continuum Solvation Models, Molecular Vibrations.				6
9	Population Analysis, Finding Transition Structures, QM/MM methods – An introduction				6
List of Text Books					
	Computational Chemistry, A.C. Norris, John Wiley.				
	Computer Programming in FORTRAN 77, R. Rajaraman, Prentice Hall.				
	Essentials of Computational Chemistry, 2 nd Edn., C.J.Cramer, Wiley				
List of Additional Reading Material / Reference Books					
	The basis of theoretical and computational Chemistry, B.M.Rode, T.S. Hofer, Wiley VCH				
	Numerical Analysis, C.E. Frogberg, Macmillan.				
	Numerical Analysis-A Practical Approach, M.J.Maron, John Wiley.				
	Numerical Methods for Scientists Engineers, H.M. Antia, Tata McGraw Hill.				

	Course Code: CHT 3025	Course Title: Nuclear Chemistry	Credits = 4		
	Semester: XX	Total contact hours: 60	L	T	P
			3	0	1
Course Outcomes (students will be able to.....)					
1	Understand the fundamental properties of nuclear radiation				
2	Understand the various analytical techniques to study the nuclear processes				
3	Identify the various applications of radioactive materials and strategies to optimize their output				
4	Recognize the health and safety aspects to ensure compliance in applicaitons				
5					
List of Prerequisite Courses					
	Undergraduate Physical Chemistry				
Course Contents (Topics and subtopics)					Reqd. hours
1	Radioactivity: Determination of half life, radioactive decay kinetics, parent-daughter decay-growth relationships, Secular and transient equilibria, Compound nucleus theory, nuclear reactions, radioactivity, induced by heavy ions				8
2	Nuclear power reactors – Nuclear fission and fusion, types of nuclear power reactors, basic features and components of a nuclear power reactor. Safety measures. Introduction to breeder reactors. Spent nuclear fuel processes and challenges involved.				10
3	Radiation Chemistry: 1. Radiation detection: Basic principles, ionization, proportional, GM counters, NaI(Tl) detectors, HPGe and Si(Li) detectors. Radiation dosimetry-units and measurement of chemical dosimeters (Fricke and ceric sulphate dosimeters). Interaction of radiation with matter. Radiation chemistry of water. A brief introduction to radiolysis of gases, liquids and solids. Industrial applications of radiation chemistry (radiation polymerization, food irradiation and radiation.				16
4	Applications of Radioisotopes: Synthesis of various useful radioisotopes, Physico-chemical, and analytical applications- isotope dilution method, activation analysis, radiometric titration, C14 dating. Medical, agricultural and industrial applications of isotopes.				16
5	Combining nuclear reactions, accelerators and production of radioisotopes. Synthesis and Chemical properties of super heavy elements				8
6	Health and Safety Aspects				2
List of Text Books					
	Principles of Radiochemistry, Eds-Sood, Ramamoorthy & Reddy (IANCAS, BARC, Mumbai)				
	Radiation Chemistry: An Overview-D. B. Naik and S. Dhanya (BARC, Mumbai)				
	Nuclear and Radiation Chemistry-Friedlander, Kennedy Macias & Miller (Wiley) 1981				
	Essentials of Nuclear Chemistry- H.J.Arnika (Wiley Eastern) 1987.				
List of Additional Reading Material / Reference Books					
	An Introduction to Radiation Chemistry-Spinks and Woods (Wiley, New York) 1990.				
	Nuclear Chemistry; New Jersey, Prentice Hall Inc., 1965.				
	Nuclear Chemistry by N.R. Johnson, E. Eichler & G. D. O Kelley-New York John Wiley & Sons. 1963.				
	Nuclear Chemistry and its applications- M. Haissinsky and D.G. Tuck				

	Course Code: CHT 3026	Course Title: Bioinorganic Chemistry	Credits = 4		
	Semester: XX		Total contact hours: 60	L 3	T 0
Course Outcomes (students will be able to.....)					
1	Understand the role of s- and p-block elements in the functioning of biomolecules				
2	Explain the functions of proteins based on the properties of the metal core				
3	Correlate the biological functions of metals and nonmetals with the physiological requirements				
4	Understand the process of photosynthesis, respiration, etc.				
List of Prerequisite Courses					
	Chemistry of Transition Metals, Biochemistry				
Course Contents (Topics and subtopics)					
			Reqd. hours		
1	Essential elements in biological systems Essential elements of life				4
	Role of essential elements: s-block elements (H, Na, K, Ca, Mg), p-block elements (B, C, Si, N, P, O, S, Se, F, Cl, Br, I), d- block elements (V, Cr, Mo, W, Mn, Fe, Co, Ni, Cu, Zn)				8
	Basic chemical processes in biological systems: Photosynthesis, Respiration, Nitrogen Fixation				8
2	Metalloproteins and Metalloenzymes Iron Heme proteins: Hemoglobin, Myoglobin, Cytochromes, Cytochrome P450				10
	Non-Heme Proteins: Hemerythrin, Methyl mono oxygenase, Ferritin Iron-Sulfur Proteins				8
	Copper Proteins: Ceruloplasmin, copper-zinc superoxide dismutase, Tyrosinase, Hemocyanin Zinc Proteins: Carbonic anhydrase, carboxypeptidases				8
3	Metal ions as charge carriers Ionophores: Valinomycin, nonactin Sodium-potassium pump				6
4	Health concern of metals and nonmetals Metal and nonmetal deficiency: Ca, Fe, I, Cu, Zn Toxic effects of metals Metals in medicine: Metals and metal compounds for diagnosis, Clinical use of chelating ligands, Coordination compounds as drugs.				6
5	Biom mineralization				2
List of Text Books					
	S. J. Lippard and J. M. Berg, Principles of bioinorganic chemistry, University Science Books, Mill Valley, 1994.				
	I. Bertini, H. B. Gray, S. J. Lippard and J. S. Valentine, Bioinorganic Chemistry, Univ. Sci. Books, Mill Valley, 1994.				
	J. A. Cowan, Inorganic Biochemistry, VCH Publishers, 1993				
List of Additional Reading Material / Reference Books					
	R. W. Hay, Bioinorganic Chemistry, Ellis Hollwood, Ltd. 1984.				
	W. Kaim and B. Schwederski, Bioinorganic Chemistry: Inorganic elements in the chemistry of life (An introduction and guide), John				

	Course Code: CHT 3027	Course Title: Developments in Organic Synthesis	Credits = 4		
	Semester: XX	Total contact hours: 60	L	T	P
			3	0	1
Course Outcomes (students will be able to.....)					
1	Understand the latest developments in the field of synthesis and catalysis				
2	Justify the use of alternative energy for carrying out organic processes				
3	Apply novel methods like electrochemical catalysis or photochemical catalysis for improved yields and selectivity				
4	Compare the role of various solvents to choose the most suitable solvent for the reaction				
5					
List of Prerequisite Courses					
	Organic Reaction Mechanism, Organic Synthesis				
Course Contents (Topics and subtopics)					Reqd. hours
1	Activation of small molecules and their applications in organic synthesis: CO, CO ₂ , CH ₄ , O ₂ , NH ₃ , and concept of C-H bond activation				13
2	New energy sources: Cavitation and sonochemistry, use of microwaves. High-pressure reactions: Principles, advantages, limitations and applications.				7
3	Microorganisms and enzymes in Organic synthesis:				4
4	New solvents: Green solvents, water, ionic liquids, supercritical fluids.				6
5	Chemicals from biomass and carbohydrates: value-added chemical synthesis, biofuels etc.				4
6	Supported reagents and catalysts: Merrifield resin and its applications. Clay supported reagents.				6
7	Multicomponent reactions: 3 component, 4-component reactions, advantages, limitations and applications.				6
8	Electrochemical synthesis: Cathodic reductions and anodic oxidations: C-C and C-X bond formation reactions, C-H bond activations reactions, cation pool methods, etc				5
9	Flow chemistry and Microreactor technology: principles, advantages, limitations and applications.				4
10	Visible light photocatalysis: oxidation reactions, reductions, C-C and C-X bond formation reactions				5
List of Text Books					
	Alternate Energy Processes in Chemical Synthesis: Microwave, Ultrasonic and Photo Activation By, V K Ahluwalia, Rajender S Varma				
	Organic Synthesis Engineering(Hardcover - 2001-02-15) by L. K. Doraiswamy				
	Visible-Light-Active Photocatalysis: Nanostructured Catalyst Design Mechanisms And Applications by Srabanti Ghosh, John Wiley, ISBN: 9783527342938				
List of Additional Reading Material / Reference Books					
	Ionic Liquids in Organic Synthesis Edited by Sanjay V. Malhotra				
	Green Solvents, Volume 6: Ionic Liquids. Paul T. Anastas, ISBN: 978-3-527-325924				
	Solid-Supported Catalysis, https://doi.org/10.1002/9781119288152.ch11				
	Activation of Small Molecules: Organometallic and Bioinorganic Perspectives, ISBN: 9783527609352				

	Course Code: CHT 3028	Course Title: Supramolecular Chemistry	Credits = 4		
	Semester: XX	Total contact hours: 60	L	T	P
			3	0	1
Course Outcomes (students will be able to.....)					
1	Recognize the specific interactions in supramolecular assemblies and effect on properties				
2	Classify the various types of supramolecular systems and design synthetic strategies for the same				
3	Identify the important applications of supramolecular assemblies in various fields				
4	Propose novel systems or modification to current systems for improved performance in applications				
List of Prerequisite Courses					
	Organic Synthesis, Stereochemistry and Spectroscopy in Organic Chemistry				
Course Contents (Topics and subtopics)					Reqd. hours
1	Nature of binding interactions in supramolecular structures: ion- ion, ion-dipole, dipole-dipole, H-bonding, cation-p, anion-p, p-p, and Van der Waals interactions.				8
2	Synthesis and structure of crown ethers, lariat ethers, podands, cryptands, spherands, calixarenes, cyclodextrins, cyclophanes, cryptophanes, carcerands and hemicarcerands., Host-Guest interactions, pre-organization and complimentarity, lock and key analogy. Binding of cationic, anionic, ion pair and neutral guest molecules, Crystal engineering of hydrogen bonded and metal-organic framework solids.				12
3	Crystal engineering: role of H-bonding and other weak interactions.				6
4	Self-assembly molecules: design, synthesis and properties of the molecules, self-assembling by H-bonding, Metal guided self- assemblies and applications ,metal-ligand interactions and other weak interactions, metallomacrocycles, catenanes, rotaxanes, helicates and knots.				12
5	Molecular devices: molecular electronic devices, molecular wires, molecular rectifiers, molecular switches, molecular logic, Design, synthesis and binding studies of synthetic receptors, Self- assembled monolayers				8
6	Relevance of supramolecular chemistry to mimic biological systems: cyclodextrins as enzyme mimics, ion channel mimics, supramolecular catalysis etc.				8
7	Examples of recent developments in supramolecular chemistry from current literature				6
List of Text Books					
	J.-M. Lehn; Supramolecular Chemistry-Concepts and Perspectives (Wiley- VCH, 1995)				
	P. D. Beer, P. A. Gale, D. K. Smith; Supramolecular Chemistry (Oxford University Press, 1999).				
List of Additional Reading Material / Reference Books					
	J. W. Steed and J. L. Atwood; Supramolecular Chemistry (Wiley, 2000)				

	Course Code: CHT 3029	Course Title: Materials Chemistry	Credits = 4		
	Semester: XX	Total contact hours: 60	L	T	P
			3	0	1
Course Outcomes (students will be able to.....)					
1	Classify the various types of nanomaterials with characteristic structures and properties				
2	List the binding and properties for the various types of nanomaterials				
3	Undertake a detailed instrumental analysis to study the structural details of such materials				
4	Model the properties of the materials on the basis of size effects				
5					
List of Prerequisite Courses					
	Chemical Dynamics, Solid State Chemistry				
Course Contents (Topics and subtopics)					Reqd. hours
1	Alloys: Ferrous and non-ferrous alloys. Interstitial and substitutional alloys, Hume-Rothery rules, Intermetallics, Shape memory alloys, Concept of phase diagrams.				4
2	Metals: metal clusters, bonding in solids- metals, semiconductors, imperfections in solids. amorphous solids. Order-disorder phenomenon in solids, Phase transitions, Solid state reactions.				8
3	Glasses & Ceramics: Glassy state, glass formers and glass modifiers. Ceramic structure. Non-oxide ceramics – carbon fibres, silicon carbide, silicon nitride, boron nitride.				2
4	Carbon materials – carbon nano tubes, fullerenes, grapheme- synthesis and applications				4
	Clays and refractory materials: Classification, structure and modifications of clays. Properties and applications of clays.				2
5	Refractories: Classification, Properties and role of bonding in properties, applications. Microscopic composites, Zeolites				2
6	Thin Films: Preparation. Physical and chemical methods of thin film formation. Epitaxial thin film growth.				3
7	Electronic and optical materials: Electronic properties of materials. Organic semiconductors and conducting materials. Electroluminescence and light emitting diodes. Piezo and ferro electric materials. Organic magnetic materials. Spin glasses. Nanomaterials- ionic conductors – solid state ionics. Organic-Inorganic hybrids. Optical and photonics materials. Luminescent materials, LCD-LED, non-linear optical materials				3
8	Liquid crystals: Classification, thermotropic/lyotropic, calamitic/discotic, nematic/smectic/columnar. Synthesis, orientation, LC displays. LC polymers.				2
11	Nanomaterials: Introduction, history, scope and perspectives: Synthesis and stabilization of nanoparticles: Chemical Reduction; Reactions in Micelles, emulsions, and dendrimers; Photochemical and radiation chemical reduction; Cryochemical Synthesis, Physical Methods				8
12	Experimental techniques in nanochemistry: Electron microscopy, X-ray and neutron diffraction, Probe microscopy,				8
13	Size effects: Models of reactions of metal atoms in Matrices; Melting point; optical spectra; Kinetic effect of chemical processes on nanoparticles; Surface of nanoparticles; Thermodynamic features of nanoparticles.				8
List of Text Books					
	Introduction to materials chemistry, Harry R. Allcock, John Wiley and Sons Inc, New York.				
	Introduction to Solids, Leonid V. Azaroff, Tata McGraw-Hill Publishing Company				

	Ltd	
	Introduction to the Physics and Chemistry of Materials, Robert J. Naumann: Boca Raton: CRC Press	
List of Additional Reading Material / Reference Books		
	Material Chemistry: Bradley D. Fahlman: Springer-Verlag, New York	
	Materials Chemistry, Fahlman B.D., Springer	
	Nanomaterials and Nanochemistry, Br'echignac C., Houdy., and Lahmani M. (Eds.)Springer Berlin Heidelberg New York. 2007.	
	Nanoparticle Technology Handbook. M. Hosokawa, K. Nogi, M. Naito and T Yokoyama (Eds.) First edition 2007. Elsevier	
	Nanotechnology Basic Calculations for Engineers and Scientists. Louis Theodore, John Wiley & Sons Inc., 2006	

	Course Code: CHT 3030	Course Title: Separation Processes	Credits = 4		
			L	T	P
	Semester: XX	Total contact hours: 60	3	0	1
Course Outcomes (students will be able to.....)					
1	Apply the concept of phase equilibria to carry out efficient distillation process				
2	Use the characteristic features of solvent extraction for effective isolation of products				
3	Understand the critical role of membranes in isolating components				
4	Utilize the concepts of separation for improving the yield of synthetic protocols				
List of Prerequisite Courses					
	Organic Synthesis				
Course Contents (Topics and subtopics)					Reqd. hours
1	Absorption, adsorption and ion exchange processes.				4
2	Distillation: Vapour-liquid equilibria. Normal and fractional distillation, batch and continuous distillation. Heat transfer in distillation. Azeotropes and separation of azeotropes. Steam distillation. Reactive distillation				8
3	Precipitation, coagulation, and flocculation. Nucleation. Normal, fractional. Sedimentation and crystallization				8
4	Sublimation				8
5	Drying				8
6	Solvent extraction: Liquid-liquid, leaching. Dissociative and reactive separations.				8
7	Filtration and centrifugation.				8
8	Membrane processes: Idea and characteristics of membranes. MF, UF, Osmosis and RO, pervaporation.				8
List of Text Books					
	Unit Operations in Chemical Engineering, McCabe and Smith				
List of Additional Reading Material / Reference Books					

Course Code: CHT 3031	Course Title: Green Chemistry	Credits = 4		
		L	T	P
Semester: XX	Total contact hours: 60	3	0	1
Course Outcomes (students will be able to.....)				
1	Identify the major environmental impact of the major synthetic processes			
2	Recognize the role of chemical exposure in the altering the human health			
3	Understand the principal role of green chemical concepts in addressing the impact of processes			
4	Design the optimum process using the green principle to minimize impact			
List of Prerequisite Courses				
	Organic Synthesis			
Course Contents (Topics and subtopics)				
				Reqd. hours
Impact on environment				
1	Chemistry of air pollution (carbon cycle, oxygen cycle, nitrogen cycle, sulphur cycle, phosphorus cycle), Air quality indices, types and sources of air pollutants, greenhouse effects			6
2	Water quality parameters, organic and inorganic contaminants, effect of chemical contaminants on ecosystem			6
Impact on human health				
3	Toxicology – definition, toxicity of chemicals, types of toxicity, factors affecting toxicity, measuring toxicity, examples			8
4	Chemical exposure, dosage, dose response, risk assessment, hazard and hazard characterisation, ADME concept			8
Introduction to Green Chemistry				
5	Nature, definition and scope of Green Chemistry, principles of Green Chemistry			6
6	Metrics for Green Chemistry: Limiting agent, yield, atom economy, reaction efficiency, E-factor Life cycle assessment: concept, details and examples			6
Green Chemistry strategies				
7	Renewable feedstocks – definition, examples, current applications, challenges and future scope Biodegradation, waste as feedstock			8
8	Energy generation from renewable feedstocks, biofuels as example – types of biofuels, solar cells, fuel cells			2
9	Catalysis, greener alternatives of catalysts, future scope			4
10	Impact of solvent, global solvent market, solvent selection, solvent replacement, neoteric solvent systems, solvent-free processes			2
11	Molecular design to contain toxicity			2
12	Sustainability, SDG by United Nations, economic aspects			2
List of Text Books				
	Green Chemistry. Theory and Practice. Paul T. Anastas and John C. Warner.			
	Green Chemistry: An Introductory Text: Edition 3 – Mike Lancaster			
List of Additional Reading Material / Reference Books				
	Introduction To Green Chemistry by Albert S. Matlack			

	Course Code: CHT 3032	Course Title: Material and Energy Balance	Credits = 4		
			L	T	P
	Semester: XX	Total contact hours: 60	3	0	1
Course Outcomes (students will be able to.....)					
1	Understand the concepts of material balance and stiochiometry				
2	Apply the concept of energy balance to chemical processes				
3	Combine the aspects material and energy balance to model processes				
4	Quantify the effect of various factors on the material and energy balance				
5					
List of Prerequisite Courses					
	Undergraduate Physical Chemistry				
Course Contents (Topics and subtopics)					
					Reqd. hours
1	Units and Dimensions. Mole concept. Compositions relationship.				8
2	Reaction stoichiometry.				8
3	Behavior of gases and vapours. Humidity and vaporization.				10
4	Simple material balance without reaction.				8
5	Material balance with chemical reaction. Complex material balance.				8
6	Energy balance associated with reactions.				10
7	Simultaneous material and energy balance. Combustion calculation.				8
List of Text Books					
	Basics principles of Chem. Engg calculations, Himmelblau				
	Chemical Process Principles Vol 1, Houghen, Watson, Ragatz				