M.Sc (Chemistry) Revised Syllabus

INSTITUTE OF CHEMICAL TECHNOLOGY

(University under Section 3 of UGC Act 1956, Elite Status & Centre of Excellence – Government of Maharashtra)

DEPARTMENT OF CHEMISTRY

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

(Accredited by the Royal Society of Chemistry, UK)

A. Preamble

Chemistry is the study of matter: its composition, properties, composition, and how some types of matter interact with other types of matter in new and interesting combinations. 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. Due to these developments, the traditional M.Sc. Chemistry courses may not be very effective and meaningful in the present age. Further, it was observed that if the Chemistry students know basic principles of Chemical Engineering, they are more effective at the application level.

On this background it was felt that a new M.Sc. programme of Chemistry was needed, which will essentially be of our interdisciplinary nature. The programme should not be compartmentalized as Inorganic Chemistry, Organic Chemistry, Physical Chemistry, etc. Some of the courses should cut across the traditional branches of chemistry and some should add value to the programme. The Institute of Chemical Technology, with advantage of having expertise in Chemical Engineering and Chemical Technology, is an appropriate Institute to run such a programme. Thus, the M.Sc. (Chemistry) programme was instituted in 2010. The course was accredited by the **Royal Society of Chemistry, U.K.,** in June 2014. With experience of last four years, the syllabus is now being revised. While revising the syllabus the recommendations of the RSC have been taken into account.

The programme has the following special features

(1) It is a semesterized and credit based programme.
(2) Chemistry will be taught as an integrated subject. It has a good blend of Inorganic chemistry, organic chemistry, physical chemistry, chemical engineering, biochemistry, materials chemistry, and interdisciplinary courses.

(3) It offers many electives and the students will opt for **four** electives in semesters III and IV.
(4) It has one course on project economics to sensitize the students with respect to economics.
(5) Through many assignments and presentations the students are expected to acquire excellent presentation and communication skills.
(6) As a component of the curriculum there is a seminar course in semester III.
(7) There is a major research component under **Project**. The students will be given research topics at the end of semester II and will work under the allotted guides.
(8) The laboratory courses in semesters I to III are open ended and enquiry driven.
(9) There will be in-semester and end-semester assessments for theory heads. The ratio of in-semester and end-semester assessment marks shall be 40:60. In the end-semester assessment there will be a formal examination. In the in-semester assessment, there will be one formal mid-semester examination carrying 20% marks. In addition, there will be a series of tests, assignments, presentations, quizzes as continuous assessment components, totally carrying 20% marks. For a practical head the ratio of in-semester and end-semester assessment marks shall be 40:60. In the end-semester assessment there will be a formal examination. The marks for the in-semester assessment will be given on the basis of the performance of the candidate during the semester.
(10) There are a few audit courses for the benefit of students.
(11) The students get opportunity to listen to experts in various fields, under endowment lecture programme. This will help them to keep abreast of recent developments in the subject areas.

Regulations Relating the Degree of Master of Science in Chemistry (M.Sc. – Chemistry)

1. Intake

20 candidates shall be admitted every year. The distribution of seats shall be as per the Institute's norms, and as per the requirement of the UGC-SAP programme.

2. Admission

(a) The candidate must have passed the post-H.S.C. 3-year degree course of Bachelor of Science with 6 units Chemistry at the third year of the course and physics as a supporting subject and Mathematics 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.
(b) The B.Sc. degree shall be of any recognized University.

(c) 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.
(d) The candidates shall have cleared the B.Sc. degree examination in one sittiing; i.e. candidates passing the B.Sc. degree in compartments shall not be eligible for the admission.
(e) The admission shall be strictly on the basis of merit in the entrance examination conducted by the Institute.

3. Programme structure

(a) The programme is a post-B.Sc., credit-based, 4-semester (2-year) programme.
(b) There will are two semesters in a year: Semester I - July to December; and semester II - December to May.
(c) Each semester will consist of 15-16 weeks of instructions, including seminars/projects/assignments/assessment.
(d) The assessment of the students shall be as per the norms of the Institute.
(e) Various activities associated with the semesters will be carried out as per the academic calendar of the Institute.
(f) The requirement of attendance of the students shall be as per the norms of the Institute.
(g) All the relevant academic Rules and Regulations of the Institute shall be applicable to the programme.
(h) In case of any difficulty regarding any assessment component of the programme, the Departmental Committee shall take appropriate decision, which will be final.
(i) **Electives:** The electives to be offered during a given semester will be declared by the Head of Departmental before the commencement of the semester. Any elective in addition to those mentioned may be offered to the students after due approval.

(j) **Project:**
  (i) At the end of the second semester, the Head of Department will assign the supervisors for the project.
  (ii) 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.
  (iii) The thesis will be evaluated by the supervisor along with one other external referee as per the norms.

4. Semester-wise pattern of the M.Sc. (Chemistry) Programme

SEMESTER I

Course No.	Title	h/ week	Credits	Marks
CHT 2201	Chemistry of main Group elements	3	3	100
CHT 2301	Organic reaction mechanism	3	3	100
CHT 2302	Heterocyclic chemistry	3	3	100
CHT 2401	Kinetics and Phase equilibria	3	3	100
CHT 2101	Instrumental methods of analysis	3	3	100
CHT 2501	Material and Energy balance	3	3	100
				600
CHP 2201	Inorganic chemistry Laboratory	4	2	50
CHP 2301	Organic chemistry Laboratory-I	4	2	50
CHP 2401	Physical chemistry Laboratory-I	4	2	50
				150
			24	**750**

SEMESTER II

Course No.	Title	h/ week	Credits	Marks
CHT 2402	Quantum Chemistry	3	3	100
CHT 2202	Chemistry of Transition metals	3	3	100
CHT 2303	Stereochemistry of Organic compounds	3	3	100
CHT 2403	Advanced thermodynamics and Electrochemistry	3	3	100
CHT 2304	Radicals, Photochemistry and Pericyclic reactions	3	3	100
CHT 2502	Fundamentals of Fluid flow and Heat transfer	3	3	100
				600
CHP 2302	Organic chemistry Laboratory II	4	2	50
CHP 2403	Physical chemistry Laboratory II	4	2	50
CHP 2403	Physical chemistry Laboratory III	4	2	50
				150
			24	**750**

SEMESTER III

Course No.	Title	h/ week	Credits	Marks
CHT 2306	Organic synthesis	3	3	100
CHT 2203	Organometallic chemistry	3	3	100
CHT 2204	Solid state chemistry, molecular symmetry, and group theory	3	3	100
CHT 2305	Advanced spectroscopy	3	3	100
CHT 2XXX	Special paper I	3	3	100
CHT 2602	Seminar	3	3	100
				600
CHP 2303	Organic Chemistry Laboratory III	4	2	50
CHP 2404	Physical Chemistry Laboratory IV Computational	4	2	50
CHP 2101	Instrumentation Laboratory	4	2	50
				150
			24	**750**

SEMESTER IV

Course No.	Title	h/ week	Credits	Marks
CHT 2404	Biochemistry	3	3	100
CHT 2603	Chemical project economics	3	3	100
CHT 2604	Catalysis	3	3	100
CHT 2XXX	Special Paper II	3	3	100
CHT 2XXX	Special Paper III	3	3	100
CHT 2XXX	Special Paper IV	3	3	100
				600
CHP 2601	Project		8	**200**
			26	**800**

Total Credits: 98, Total Marks: 3050

Special Papers

CHT 2311. Natural Products
CHT 2312. Polymer Chemistry
CHT 2611. Surface and Interfacial Chemistry
CHT 2411. Computational Chemistry
CHT 2211. Nuclear Chemistry
CHT 2212. Bioinorganic Chemistry
CHT 2313. Developments in Organic Synthesis
CHT 2511. Unit Processes in Organic Synthesis
CHT 2213. Nanochemistry
CHT 2612. Supramolecular Chemistry
CHT 2214 Materials Chemistry
CHT 2512 Separation Processes
CHT 2513 Industrial Engineering Chemistry

Course code legend:

CHT- Theory course CHP- Practical course

XXXX = ABCD

A: 1- UG; 2- PG
B: 1-AC; 2 – IC; 3- OC; 4- PC; 5- CE; 6- Interdisciplinary
C: 0 – Core; 1- Special Paper
D: Individual course No. under B

B. Detailed Syllabus of the M.Sc.(Chemistry) Programme

SEMESTER I

CHT 2201. Chemistry of Main Group Elements

Unit	Content	h
1	**s-block elements:** Salient features of hydrides, solvation and complexation tendencies, function in biosynthesis.	4
2	**p-block elements:** Hydrides, oxides, oxyacids, and halides, hydrides of boron - diborane and higher boranes, borazine, borohydrides, fullerenes, carbides tetrasulfur tenitride.	6
3	**Streochemistry and bonding in main group elements:** VSEPR, Walsh diagrams (tri- and penta-atomic molecules), dπ-pπ bonds, Bent rule and energies of hybridization. Simple reactions of covalently bonded molecules.	3
4	**Lanthanides:** Occurrence and isolation, separation. Electronic structure, oxidation states. Lanthanide contraction and ionic radii. lanthanide compounds and complex formation.	5
5	**Actinides:** General features and chemistry of actinides, chemistry of separation of Np, Pu and Am from U. Similarities between	4
6	**Silicones and Phosphazenes:** Silicones and phosphazenes as examples of inorganic polymers, nature of bond in triphosphazines. Later actinides and later lanthanides.	3
7	**Metal clusters:** Higher boranes, carboranes, metalloboranes and metallocarboranes, metal carbonyls and halide clusters, compounds with metal-metal multiple bonds.	5

CHT 2301. Organic Reaction Mechanism

Unit	Content	h
1	**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.	4
2	FMO theory and its applications.	3
3	Acid-Base concepts. Solvent effects.	2
4	Tautomerism - including ring-chain and valence tautomerism.	1
5	**Aromaticity:** Criteria of aromaticity. Huckel MO theory, Frost-Muslin geometrical interpretation. Carbocyclic systems, ferrocenes, azulenes, annulenes, tropylium ion, fulvenes, sydnones. Recent ideas of aromaticity.	2

6	Aromatic electrophilic and nucleophilic substitution, benzyne intermediate	2
7	Thermodynamic and kinetic control.	1
8	**Substitution:** S_N1, S_N2, S_Ni, S_N',S_NCA reactions, NGP	4
9	**Elimination:** E_1, E_2, E_1cB, Zaitsev and Hoffmann elimination	2
10	**Addition reaction:** Hydroxylation and dihydroxylation of olefins	2
11	**Chemistry of enolate:** Generation and reactions.	2
12	**Reaction intermediates:** Ketenes, carbenes, nitrenes, singlet oxygen: Generation, structure and reactions.	3
13	**Tetrahedral mechanism:** Esterification and hydrolysis of esters.	2

CHT 2302. Heterocyclic Chemistry

Unit	Content	h
1	**Nomenclature:** Nomenclature of heterocyclic compounds- Trivial, Hantzch-Widman, Replacement. Nomenclature of mono and polycyclic compounds. Polarity, tautomerism, aromaticity, electrophilic substitution.	5
2	**Small rings:** aziridines, thiirane, azetidine, oxetane, thietanes	3
3	**Five membered:** Diazoles, oxazoles and thiazoles.	7
4	**Six membered:** Diazines, triazenes, pyranes and pyrones	7
5	**Seven membered:** Diazepines	2
6	**Fused ring:** Benzofurans, benzopyrones, benzodiazepines, indole, quinolines and isoquinolines, purines	6
	Assignment topics: heterocyclic compounds as drugs, dyes, optical brighteners, perfumes, etc	

CHT 2401 Kinetics and Phase Equilibria

Unit	Content	h
1	**Kinetics:** kinetics of gas phase reactions- simple and complex reactions - parallel, reversible and consecutive reactions, kinetics of chain reactions, branched chain reactions and explosion limits Temperature effect on reaction rates, theories of reaction rates Reactions in molecular beams .	10
2	**Homogeneous reactions:** Kinetics of homogeneous acid base reactions, auto catalytic and oscillatory reactions, kinetics of fast reactions, solvent effects and diffusion controlled reactions.	10
3	Phase equilibria and phase diagrams of two and three component systems, thermodynamic description of phase transitions, lambda transitions- first order and second order phase transitions.	10

CHT 2101. Instrumental Methods of Analysis

Unit	Content	h
1	**Basics:** Statistical and mathematical operations in Chemistry, Units, dimensions and concentration, Errors and evaluation, Solid Sampling. Precision and Accuracy, Deviations, T- F- and C-tests, Regression analysis, Instrument calibration and validation. Certified reference materials.	7
2	**Flame spectrometry:** FES, AAS, AFS,	3
3	**Molecular luminescence:** Fluorescence, Phosphorescence, Chemical/Bio Luminescence	4
4	**Electroanalytical method:** voltmetry, cyclic voltmetry, coulometry, ion selective electrodes and sensors, polarography, anodic/cathodic stripping, electroless deposition	4
5	**Diffraction techniques:** Powder X-ray diffraction methods. Neutron diffraction	2
6	**Surface characterization:** SEM, TEM, AFM	2
7	**HPLC:** Principles, columns including chiral columns, detectors. Ion exchange chromatography, exclusion chromatography, gel permeation chromatography, HP-TLC	5
8	**Emission:** Flame photometry, ICP, Ark-Spark spectra, Phosphorescence, XRF	3

Note: The techniques should be discussed with emphasis on applications

CHT 2501. Material and Energy Balance

Unit	Content	h
1	Units and Dimensions. Mole concept. Compositions relationship.	4
2	Reaction stoichiometry.	4
3	Behavior of gases and vapours. Humidity and vaporization.	4
4	Simple material balance without reaction.	5
5	Material balance with chemical reaction. Complex material balance.	5
6	Energy balance associated with reactions.	4
7	Simultaneous material and energy balance. Combustion calculation.	4

Practicals:

CHP 2201 Inorganic Chemistry Laboratory-I

Preparation and characterization of inorganic complexes comntaining 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.

CHP 2301 Organic Chemistry Laboratory-I

Purification techniques: Crystallization, distillation – simple and fractional, sublimation, steam distillation, chromatography – TLC and column. Purity checking through physical constants and TLC.
Separation techniques: Separation of multicomponent mixtures through Physical and chemical methods.

CHP 2402 Physical Chemistry Laboratory-I

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.

Safety in Chemical Laboratory: The students should be given a safety manual and are expected to get acquainted with all the relevant safety norms. In each laboratory respective training will be imparted and the students will be evaluated through tests and assignments.

SEMESTER II

CHT 2402. Quantum Chemistry

Unit	Content	h
1	**Mathematical review:** Matrices and determinants, polar, cartesian and spherical coordinates, Legendre and Laugurre polynomials, Taylor and McLaurin series, linear and Hermitian operators	3
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	2
3	**Applications of Schrodinger equation to simple systems** – particle in a box, harmonic oscillator, rigid rotor	3
4	**H and H like atoms**- two particle problem, Schrodinger equation in spherical coordinates, representation of orbitals, radial and angular plots, probability functions	5
5	**Approximation methods**- variation and perturbation theorems	3
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	6
7	**Chemical bonding in diatomic molecules-** Born-Oppenheimer approximation, LCAO and MO theory- H_2^+ in ground electronic 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.	5
8	**Chemical bonding in polyatomic molecules**- semi empirical method-Huckel theory, application to simple pi systems, An introduction to *ab initio*, DFT and MM methods.	3

CHT 2202. Chemistry of Transition Metals

Unit	Content	h
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.	3
2	**Coordination compounds:** Werners coordination theory and its experiments verification, effective atomic number concept, chelates, nomenclature of coordination compounds, isomerism in	4

	coordination compounds, valence bond theory (VBT) of transition metal complexes.	
3	**Electronic spectra of transition metal complexes:** Types of electronic transition, selection rules for d-d transitions, spectroscopic ground stares, spectrochemical series, Orgela and Tanabe-Sugano diagrams for transition metal complexes (d^1-d^9 states), calculations of Dq, B and beta parameters, change transfer spectra, discussion of the electronic spectrum of $[Ti(H_2O)_6]^{3+}$ complex ion.	4
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 *ueff* 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.	4
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.	3
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.	3
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.	4
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 one electron transfer reactions, outer sphere type reactions, cross reactions, inner sphere type reactions.	5

CHT 2302. Stereochemistry of Organic Compounds

Unit	Content	h
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 tentracoordinate centres – N, S, Si, P, As. (vi) allenes, spiranes, biphenyls, ansa compounds, paracyclophanes, alkylidene cycloalkanes	8
2	**Strain and strain energy,** polycyclic compounds	2
3	**Resolution methods:** Types of racemic mixtures, resolution of racemic mixtures	1
4	**Conformational analysis:** Acyclic and cyclic compounds. Decalin	3
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. Asymmetric reactions: aldol reaction, Michael reaction, Sharpless epoxidation, dihydroxylation, oxidations and reductions aminohydroxylation; Jakobson epoxidation, Hydrogenation, Diels-Alder reaction. Chiral borane reagents. Asymmetric catalysis- Grubb's catalyst, Wilkinson's catalyst.	8

CHT 2303. Radicals, Photochemistry, and Pericyclic Reactions

Unit	Content	h
1	**Radicals**	
	1.1 Radicals: Generation of radicals. Nucleophilic and electrophilic radicals. Characteristic reactions - Free radical substitution, addition to multiple bonds.	2
	1.2 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: SNAr reactions. Hoffman-Loffler-Freytag reaction.	6
2	**Photochemistry**	
	2.1 Excited state: Joblonski diagram - Fluorescence, phosphorescence. Principle of energy transfer. Chemical reactivity of electronically excited molecules - orbital character,	2

	acidity, redox, etc. Exciplex formation. Triplet sensitization and delayed fluorescence	
	2.2 Photosensitized reactions, chemiluminiscence. Photosensitization, quenching, quantum efficiency and quantum yield.	2
	2.3 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, adamantine, etc. Flash photolysis and lasers	6
3	**Pericyclic reactions**	
	3.1 Types: Thermal and photochemical. Classification of pericyclic reactions. Cycloaddition, electrocyclic reactions, sigmatropic rearrangement, 1,3-dipolar reactions, [3,3] shifts. Group transfer reactions.	3
	3.2 Theories of pericyclic reactions: Huckel molecular orbitals (i) Conservation of orbital symmetry (ii) FMO (iii) Aromatic transition state. Woodward-Hoffmann rules. **3.3 Cycloaddition reactions:** Diels-Alder reaction – Alder rule, endo preference, Lewis acid catalysis. [2+2] cycloaddition of ketenes, dipolar cycloaddition, cheletropic reactions; Photochemical reactions.	5
	3.4 Electrocyclic reactions: ring opeing of cyclobutenes, ring closure of hexatrienes, cyclopropyl halide sovolysis; charged systems.	3
	3.5 Sigmatropic rearrangements: [1,n] H-atom shifts, Cope and Claisen rearrangements, ene reaction.	1

CHT 2402 Advanced Thermodynamics and Electrochemistry

Unit	Content	h
1	**Non-equilibrium Thermodyamics** Thermodynamics of irreversible processes, conversion of mass and energy in open and closed systems, non adiabatic processes, generalized forces and fluxes, Clausius inequality Nonequilibrium thermodynamics: Postulates and methodologies, linear laws.	7
2	**Molecular Thermodynamics** Concepts of micro states and micro configuration, degeneracy. Statistical thermodynamics- probability and entropy, distribution laws of MB, FD and BE, partition functions- rotational, vibrational and translational partition functions of diatomic molecules, calculation of thermodynamic functions and equilibrium constants, theories of specific heats of solids.	8
3	**Electrochemistry**	4

	3.1. Electrochemistry of solutions- Debye Huckel theory and Debye-Huckel equation, ionic strength, activity and activity coefficient, dependence of activity coefficient on ionic strength. Solvent interactions, heats of hydration, hydration number, pair formation, Bjrreum theory.	
	3.2. Electrochemical cells and electrochemical potentials, applications of emf measurements to determine dissociation constants of weak acids, solubility product, stability constant and formula of a complex, liquid junction potential, mean ionic coefficient.	4
	3.3. Electrical double layer, electro capillarity, electrokinetic phenomena, zeta potential and its applications.	2
	3.4 Kinetics of electrode reactions – One and two electron transfer reactions,	2
	3.5 Electrochemical synthesis.	1
	3.6 Fuel cells and batteries	2

CHT 2502. Fundamentals of Fluid Flow and Heat Transfer

Unit	Content	h
1	**Fluid characteristics:** Viscosity, density, velocity, pressure and pressure difference, surface tension. Newtonian and non-newtonian fluids. Concept of drag. Raynold number.	4
2	**Types of flow:** Laminar and turbulent flow. Co- and Counter flow	2
3	Flow characteristics, flow measurement, Effect of geometry on fluid flow.	3
4	Fluid passed immersed bodies. Flow through pipes. Mixing in fluids	3
5	Transportation of fluids. Pumps. Metering of fluids.	2
6	Agitation and mixing of liquids. **Mass Transfer**: Mass transfer effects on reaction kinetics and processes. Agitation and mass/heat transfer. Surface transfer phenomenon.	4
7	**Heat transfer:** Concept of heat transfer. Heat transfer to fluids with and without phase change. Mechanism of Heat transfer: Conduction and convection.	4
8	Evaporation, boiling, refrigeration.	3
9	Heat exchangers, heat transfer media	3
10	Types of reactors	2

Practicals:

CHP 2302 Organic Chemistry Laboratory-II

One step organic synthesis involving electrophilic and nucleophilic reactions of aliphatic and aromatic compounds, oxidation-reduction reactions, condensation reactions, eliminations reactions, catalytic reactions, and use of new reagents.

CHP 2402 Physical Chemistry Laboratory-II

Determination of transport number, experiments based on cyclic voltametry and polarography, experiments based on surface/interface chemistry and macromolecules. thermodynamics (L-L, V-L equilibria), phase diagrams (L-L system).

Experiments to determine rate laws and rate constants, oscillatory and clock reactions, kinetic measurements through optical rotation measurements. Experiments based on surface tension and surfactant aggregates.

Nuclear Chemistry Experiments:

1. Determination of energy resolution of a NaI(Tl) detector
2. Determination of gamma-ray attenuation coefficients
3. Determination of operating voltage of a GM counter and testing statistical nature of radioactivity

(Original source of experiments: Experiments in Radiochemistry by D. D. Sood, S. B. Manohar and A. V. R. Reddy)

CHP 2403 Physical Chemistry Laboratory -III

Experiments based on fluid flow (flow through horizontal pipe and through fittings, rotameters, orifice meter, terminal settling velocity), heat transfer (double pipe heat exchanger), mass transfer (differential distillation, L-L extraction), thermodynamics (L-L, V-L equilibria), phase diagrams (L-L system), process control (tanks in series).

SEMESTER III

CHT 2304. Organic Synthesis

Unit	Content	h
1	Disconnection approach and retrosynthetic analysis. Planning of multistep synthesis. Concepts of synthones, retrones and synthetic equivalents. Generation of structural complexity using tandem and cascade processes.	4
2	**Functional groups:** Their reactivity profile, interconversions and protection. Umpolung,	2
3	**Ylides**: Ylides of P and S. Wittig reaction and its modifications,	2
4	**Enamines:** Synthesis, reactivity and synthetic importance.	2
5	**Ring cyclization methods:**	
6	**Reduction:** Catalytic hydrogenation. Dissolving metal reductions. Hydride transfer reagents. Complex hydrides including nucleophilic, electrophilic and radical reducing agents. Organo boranes. MVP reduction.	4
7	**Oxidation:** Cr,Os, Ti, Fe and Mn reagents, per acids and peroxides, Oxidation by ozone and oxygen, Swern oxidation. Bayer Viliger oxidation	3
8	**Selected organic reagents:** TMSC/I, TBTH, DCC, DDQ, TCQ, CAN, NBS, DIBAL,PTC, Crown ethers, SmI_2, SeO_2 Corey-Chaykowsky reagent, DABCO, Gilmans reagent, Lawesson reagent, Simmon Smith reagent.	4
9	**Selected name reactions:** Hoffmann-Loffler-Fritag reaction, Sharp reaction, Paterson reaction, Heck reaction, McMurry coupling reaction, Suzuki reaction, Birch reduction, Woodward-Prevost reaction, Mukaiyama esterification, Mitsunobu reaction. Finkelstein reaction, Buchwald-Hartwig amination, McMurry coupling, Baylis-Hilman reaction, Corey-Fuchs reaction , Ritter reaction, Tsuji-Trost allylic alkylation.	5
10	**Rearrangements:** Favorskii reaction, Curtius Lossen, Benzil-Benzilic acid rearragentment, Steven, Shapiro, Tiffenev-Demyanov, Benzidine rearrangement, Baker-Venkatraman rearrangement, Ireland-Claisen rearrangement, Wittig rearrangements.	4
	Assignment topics: Strained molecules: Prismanes, cubane, and other strained molecules. Adamantane **Nonconventional energy sources:** Microwaves and ultrasound based synthesis	

CHT 2203. Organometallic Chemistry

Unit	Content	h
1	**Recapitulation:** Werner complexes, *trans* effect, Soft versus Hard ligands, Crystal Field and ligand field, Back bonding, Electroneutrality, Types of ligand	2
3	**General Properties of Organometallic Complexes**: 18-electron rule and its limitation, Electron counting in reactions, Oxidation state, coordination number and geometry, Effects of complexation, Differences between metals, Outer-Sphere coordination	2
4	**Metal Alkyls, Aryls, and Hydrides and Related**: σ-Bonded ligands, Transition metal alkyls and aryls, Related σ-bonded ligands, Metal hydride complexes, σ-complexes, Bond strengths for classical σ-bonding ligands	3
5	**Carbonyls, Phosphine Complexes, and Ligand Substitutio Reactions**: Metal complexes of CO, RNC, CS, and NO, Phosphines and related ligands, Dissociative substitution, Associative mechanism, Redox effects, the I Mechanism, and rearrangements in substitution, Photochemical substitution, Steric and Solvent effects in substitution	4
7	**Complexes of π-Bound Ligands:** Alkene and Alkyne complexes allyl complexes, Diene complexes, Cyclopentadienyl complexes, Arenes and other alicyclic ligands, Metalacycles and isoelectronic and isolobal replacement, Stability of polyene and polyenyl complexes	3
8	**Oxidative Addition and Reductive Elimination:** Concerted Additions, S_N2 reactions, Radical mechanisms, Ionic mechanisms, Reductive elimination, σ-Bond metathesis, Oxidative coupling and Reductive cleavage.	2
9	**Insertion and Elimination**: Reactions iInvolving CO, Insertions Involving alkenes, Other insertions, α, β, γ, and δ Eliminations	2
10	**Nucleophilic and Electrophilic Addition and Abstraction:** Nucleophilic addition to CO, Nucleophilic addition to polyene and polyenyl ligands, Nucleophilic abstraction in hydrides, alkyls, and acyls, Electrophilic addition, Electrophilic abstraction of alkyl groups, Single-electron transfer pathways, Reactions of organic free radicals with metal complexes	3
13	**Physical Methods in Organometallic Chemistry**: Isolation, ^{1}H, ^{13}C and ^{31}P NMR, Dynamic NMR, Spin saturation transfer, T1 and the NOE, Isotopic perturbation of resonance, IR Spectroscopy, Crystallography, Other methods	3
14	**Metal–Ligand Multiple Bonds:** Carbenes, Carbynes, Bridging Carbenes and Carbynes, N-Heterocyclic carbenes, Multiple bonds to heteroatoms, Applications of organometallic chemistry	3

	Alkene metathesis; Dimerization, oligomerization, and polymerization of alkenes, Activation of CO and CO_2, CH.	
	Clusters and the Metal–Metal Bond: Structures, The Isolobal analogy, Synthesis, Reactions, Giant Clusters and Nanoparticles, Giant Molecules, Metal alkyls aryls, and hydrides,	2
	Paramagnetic, High-Oxidation-State, and High-Coordination-Number Complexes: Magnetism and spin states, Polyalkyls, Polyhydrides, Cyclopentadienyl complexes, f -Block complexes	1

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CHT 2204 Solid state Chemistry, Molecular Symmetry, and Group Theory

Unit	Content	h
1	**Solid state chemistry**	
	1.1 An introduction to crystal structure- lattice types and unit cells, Millar indices, close packing	**2**
	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	**3**
	1.3 Characterization of solids- diffraction methods- X ray , electron and neutron diffraction, electron microscopy, EDAX , XANES techniques	**3**
	1.4 Bonding in solids- Ionic crystals, lattice energy of ionic crystals, metallic crystals. Band theory and electronic conductivity, Zone theory- Brillioun zones, k – space, Fermi surfaces and density states	**2**
	1.5 Properties of solids- metals, semi conductors and p-n junctions , super conductors- theory and applications , ionic conductivity, photo conductd ivity, defects in solids, non stoichiometry Optical properties- lasers, light emitting diodes Magnetic and dielectric properties- types of magnetic properties, magento resistance	**5**
2	**Molecular symmetry and Group theory**	
	2.1 Introduction to molecular symmetry – symmetry elements and operations.	2
	2.2 Classification and assignment of point groups to Inorganic molecules, multiplication tables and matrix representation – unitary and reducible representations	3
	2.3 The great orthoganality theorem, character tables	3
	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.	4
	2.5 Application of Group Theory to vbrational spectroscopy: A brief idea about Infrared and Raman scattering spectroscopy, vibrational modes as basis of group representations	3

CHT 2305. Advanced Spectroscopy

Unit	Content	h
1	**UV-VIS spectroscopy -** Woodward rules, aromatic and heterocyclic compounds	3
2	**IR and Raman spectroscopy:** FT technique, group frequencies, vibrational coupling. **NIR spectroscopy**. New applications. Scattering phenomena and **Raman spectroscopy**.	4
3	**NMR spectroscopy: H1 NMR:** Chemical shifts and factors affecting the same, spin-spin coupling of different systems. Long range coupling, Simplification of complex spectra. Pulse technique. **C13 NMR:** Basics, Off-resonance, APT and DEPT. **F19 and P31 NMR.** **2D NMR techniques –** COSY, HETCOR, NOE. Solid state NMR.	14
4	**Mass spectrometry:** Basics. Different techniques. Isotopic abundance. Fragmentation. Rearrangement of ions.	6
5	**Hyphenated techniques:** GC-MS, LC-MS, HP-TLC	3

Special Paper I CHT 2X1X

CHT 2602. Seminar

Seminar topics will be given at the beginning of the second year (Semester III) by the Head of Department. Faculty mentors will be assigned to the students to guide them. Students are expected to do literature survey and do critical review of the literature. A report will be prepared in the prescribed format, with approval from the mentor. The students will submit the report at the end of the third semester and give a seminar; as per the schedule. The report and the seminar will be evaluated by a committee constituted for the purpose; with the mentor as the internal examiner.

Practicals:

CHP 2303 Organic Chemistry Laboratory-III

Multistep synthesis. Experiments based on Green Chemistry principles, natural products chemistry and medicinal chemistry.

CHP 2101 Instrumentation Laboratory

Use of instrumental methods: GC, UV-VIS, IR, HPLC, MS, GC-MS, XRD. Interpretation of spectral data.

CHP 2404 Physical Chemistry Laboratory IV

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 Transition states, Ab initio and DFT calculations

Learning Programming language – Python: Introduction to Python GUI, Arithmatic 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

SEMESTER IV

CHT 2404. Biochemistry

Unit	Content	h
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.	4
2	**Nucleic acids:** Conformation and function of DNA and RNA, genetic code, mutation, recombinant DNA, DNA synthesis, DNA biosynthesis and related drugs.	5
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.	6
4	Structure and biological functions of - coenzyme A, thiamine pyrophosphate, pyridoxyl phosphate, NAD+, NADP+, FAD, FMN, flavin dinucleotide, vit B12.	4
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.	4
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.	5
7	**Lipids:** Structure, classification, characterization, metabolism	2

CHT 2603. Chemical Project Economics

Unit	Content	h
1	Meaning of project & economics. Introduction to types of project & Elements of management of project. Transfer price.	3
2	**Introduction to**: Elements of project cost, Cost of production, Project financing, Interest, Loan repayment, Depreciation and Economy of scale.	14
3	**Estimate of working results:** Gross profit, Operating profit, Taxable income, Corporate tax, Dividend.	3
4	**Project evaluation**: Pay back , Break even, Weighted average cost of capital, Discounted profit flow analysis: Present value analysis, Profitability Index, and IRR.	5
5	Demand curve, marketing	3
6	Feasibility report, Annual report	2

CHT 2604. Catalysis

Unit	Content	h
1	**Types of catalysis:** Heterogeneous and Homogeneous catalysis. Catalytic cycles. TON, TOF	1
	Catalyst preparation: Bulk and supported catalysts, deactivation and regeneration.	2
	Characterization of catalysts: Surface area, surface acidity and basicity, XPS, UPS, AES, EXAFS, XANES, XRD TPD.	3
2	**Heterogeneous catalysis:** Adsorption isotherms, kinetics of heterogeneous catalytic reactions, structure of adsorbed species. 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.	9
4	**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, 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	15

Special Paper II CHT 2X1X

Special Paper III CHT 2X1X

Special Paper IV CHT 2X1X

CHP 2601 Project

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.

C. SPECIAL PAPERS

CHT 231X. Natural Products

Unit	Content	h
1	**Steroids:** Occurance, structure, classification, biological role. Important structural and stereochemical features of cholesterol, ergosterols, bile acids, steroidal hormones. Synthesis of 16-DPA from cholesterol, synthesis of commercially important steroids from 16-DPA, synthesis of Taxol.	9
2	**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.	10
3	**Plant pigments:** General structural features, occurance, isolation, biological importance, and applications of - carotenoids, anthocyanins, flavones. Structure determination and synthesis of B-carotene.	3
4	**Prostaglandins:** Classification and biological importance. Structure determination and synthesis of PGE1 and PGF1.	2
5	Insect pheromones: Structural features, classification, and importance. Synthesis of bombycol and gossyplure.	2
6	Plant growth regulators and insect growth regulators: genral idea, structure, examples and applications. Synthesis of pyrenthrin.	1
7	**Antibiotics:** Classification. B-lactam antibiotics. Penicillins and cephalosporins. en-dyne-antibiotic.	3
	Assignment topics: Fascinating Organic synthesis: Reserpine, Longifoline, Grisofulvin, Quinine, Oestrone, B-vetivone, Colchicine	

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CHT 231X. Polymer Chemistry

Unit	Content	h
1	**Monomers:** Their sources and synsthesis	1
2	**Methods of polymerization:** Bulk, Solution, Supsension, Emulsion, Addition, Melt, Condensation.	2
3	**Mechanisms of polymerization:** Ionic and coordination polymerization. Step-Grown vs chain growth. Degree of polymerization.	2
4	**Properties of polymers:** Viscocity, end-group analysis, hardness, abrasion resistance Structure and properties: Morphology and crystallinity, Molecular weight distribution-Number and weight average molecular weight. Polydispersity,	8

	crystallinity. Glassy state - Glass transition temperature Tm and Tg. Stereochemistry.	
5	**Additives in polymers:** Plasticizers, stabilizers, antioxidants, fillers, pigments, etc.	2
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	1
8	**Advanced polymers**	4

CHT 261X. Surface and Interfacial Chemistry

Unit	**Content**	**h**
1	Concept of surface free energy and surface tension, interfacial tension and interfacial free energy, surface excess.	**2**
2	**Liquid surfaces**	
	2.1 Thermodynamics of liquid surfaces: Gibbs adsorption isotherm, spreading coefficient and wetting phenomena.	**2**
	2.2 Thermodynamics of curved surfaces: Young, Laplace, Kelvin, and Thomson equations.	**2**
	2.4 Potentials of interfaces, interfacial viscosity. Insoluble monolayers, LB films and molecular self assembly.	**4**
	2.4 Bubbles and foams, homogeneous and heterogeneous nucleation.	**2**
3	**Solid- liquid interfaces:** Work of adhesion and cohesion, wetting and contact angles, adsorption from solution at solid/ liquid interfaces, critical surface tension.	**3**
4	**Surfactants** Introduction: General structure, types, nomenclature Surfactant aggregates – Factors affecting aggregational behaviour	**4**
	Emulsions, microemulsions, gels, foams, colloids.	**4**
	Synthesis of surfactants: Synthesis of hydrophobes, functionalisation of hydrophobes	**3**
	Applications of surfactants, Biosurfactants and biodegradable surfactants, Mixed surfactant systems	**3**
5	Hydrotropes: Nature, structure, behavior, applications	**1**

CHT 241X. Computational Chemistry

Unit	Content	h
1	Introduction to Computational Chemistry, Basic concepts	2
2	Molecular Mechanics methods, Optimization methods, Defining Geometry and Z-matrix	4
3	Electronic structure - methods: Schrodinger Equation, Born–Oppenheimer Approximations, SCF Theory, Energy of Slater Determinant, Koopmans' Theorem, Basis Set Approximation, Basis Sets	6
4	Hartree-Fock Approximation, Correlation, Moeller-Plesset Perturbation Theory, Configuration Interaction, Multi-configurational Self-consistent Field	4
5	Semiempirical Methods	2
6	Density Functional Theory	4
7	Applications in Drug Designing, Statistics and QSAR, Applications in Catalysis	2
8	Simulation Techniques: Monte Carlo Methods, Molecular Dynamics,Solvation Models, Continuum Solvation Models, Molecular Vibrations.	4
9	Population Analysis, Finding Transition Structures, QM/MM methods – An introduction	2

CHT 221X. Nuclear Chemistry

Unit	Content	h
1	**Radioactivity:** Determination of half life, radioactive decay kinetics, parent-daughter decay-growth relationships, Secular and transient equilibria, Compund nucleus theory, nuclear reactions, radioactivity, induced by heavy ions	4
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.	5
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.	9
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.	7

5	Combining nuclear reactions, accelerators and production of radioisotopes. Synthesis and Chemical properties of super heavy elements	3
6	Health and Safety Aspects	2

CHT 221X Bioinorganic Chemistry

Unit	Content	h
1	**Essential elements in biological systems** Essential elements of life 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) Basic chemical processes in biological systems: Photosynthesis, Respiration, Nitrogen Fixation	 1 4 4
2	**Metalloproteins and Metalloenzymes** Iron Heme proteins: Hemoglobin, Myoglobin, Cytochromes, Cytochrome P450 Non-Heme Proteins: Hemerythrin, Methyl mono oxygenase, Ferritin Iron-Sulfur Proteins Copper Proteins: Ceruloplasmin, copper-zinc superoxide dismutase, Tyrosinase, Hemocyanin Zinc Proteins: Carbonic anhydrase, carboxypeptidases	 3 2 1 2 1
3	**Metal ions as charge carriers** Ionophores: Valinomycin, nonactin Sodium-potassium pump	 2 2
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.	 1 2 1 3
5	Biomineralization	1

CHT 231X. Developments in Organic Synthesis

Unit	Content	H
1	**Activation of small molecules:** CO, CO_2, O_2, CH_4, NH_3. C-H bond activation	5
2	**New energy sources:** Cavitation and sonochemistry, use of microwaves. Microorganisms and enzymes in Organic synthesis High pressure reactions	4
3	**New solvents:** Water, ionic liquids, supercritical fluids, green	4

	solvents	
4	Chemicals derived from methane, carbon monoxide, carbon dioxide, synthesis gas, carbohydrates, and biomass.	5
5	**Supported reagents and catalysts:** Merrifield resin and its applications. Clay supported reagents.	4
6	**Electrochemical synthesis:** Cathodic reductions and anodic oxidations	4
7	**Multicomponent reactions.**	3
8	Microreactor technology	1

CHT 251X. Unit Processes in Organic Synthesis

Unit	Content	h
1	Applications of Thermodynamics in Unit processes; Chemical kinetics, Chemical process kinetics	4
2	**Unit processes in** – Nitration, amination by reduction of nitro group, halogenation, sulphonation, sulfation, amination by ammonolysis, oxidation, hydrogenation, hydrocarbon synthesis, hydroformylation, esterification, hydrolysis, alkylation.	26

CHT 261X Nanochemistry

Unit	Content	h
1	Introduction, history, scope and perspectives	2
2	Synthesis and stabilization of nanoparticles: Chemical Reduction; Reactions in Micelles, emulsions, and dendrimers; Photochemical and radiation chemical reduction; Cryochemical Synthesis, Physical Methods	4
3	Experimental techniques in nanochemistry: Electron microscopy, X-ray and neutron diffraction, Probe microscopy,	6
4	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.	10
5	**Applications of nanoparticles: In -**industry, medical field, research. Environmental issue. Toxicity and biosafety in application of nanoparticles	8

CHT 261X Supramolecular chemistry

Unit	Content	h
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.	4
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.	6
3	Crystal engineering: role of H-bonding and other weak interactions.	3
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.	6
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	4
6	Relevance of supramolecular chemistry to mimic biological systems: cyclodextrins as enzyme mimics, ion channel mimics, supramolecular catalysis etc.	4
7	Examples of recent developments in supramolecular chemistry from current literature	3

CHT 221X. Materials Chemistry

Unit	Content	h
1	**Alloys:** Ferrous and non-ferrous alloys. Interstitial and substitutional alloys, Hume-Rothery rules, Intermetallics, Shape memory alloys, Concept of phase diagrams.	3
2	**Metals**: metal clusters, bonding in solids- metals, semiconductors, imperfections in solids. amorphous solids. Order-disorder phenomenon in solids, Phase transitions, Solid state reactions.	3 6
3	**Glasses & Ceramics:** Glassy state, glass formers and glass modifiers. Ceramic structure. Non-oxide ceramics – carbon fibres, silicon carbide, silicon nitride, boron nitride.	2
	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.	4

	Refractories: Classification, Properties and role of bonding in properties, applications. Microscopic composites **Zeolites**	
5	**Dyes:** Functional dyes, Chemiluminescence and fluorescence Photochromic and solvachromic dyes	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.	4
8	Luminescent materials, LCD-LED, non-linear optical materials	2
10	**Supramolecular chemistry:** Molecular complexes. Host-Guest chemistry and Molecular recognition. Crown ethers, cryptands, cyclodextrins, calixarenes, cavitands. Supramolecular devises. Self assemblies. Applications in drug delivery and separation science.	5
11	**Liquid crystals:** Classification, thermotropic/lyotropic, calamitic/discotic, nematic/smectic/columnar. Synthesis, orientation, LC displays. LC polymers.	2

CHT 251X Separation Processes

Unit	**Content**	**h**
1	Absorption, adsorption and ion exchange processes.	2
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	6
3	Precipitation, coagulation, and flocculation. Nucleation. Normal, fractional. Sedimentation and crystallization	4
4	**Sublimation**	2
5	**Drying**	2
6	**Solvent extraction:** Liquid-liquid, leaching. Dissociative and reactive separations.	6
7	Filtration and centrifugation.	2
8	**Membrane processes**: Idea and characteristics of membranes. MF, UF, Osmosis and RO, pervaporation.	6

CHT 251X Industrial Engineering Chemistry

Unit	Content	h
1	Types of Chemicals. Status of global and Indian Chemical Industry.	2
2	Operation and Processes in Petrochemical Industry	2
3	**Coal:** Types. Carbonization, liquefaction, gasification.	4
4	Physicochemical principles of manufacture of important inorganic and organic bulk chemicals such as sulphuric acid, nitric acid, ammonia, chlorine, sodium hydroxide, sodium carbonate, urea, ethylene, propylene, butadiene, acetylene, BTX, alkyl benzenes, vinyl chloride, phenol, styrene, esters, ethylene oxide, phthalic acid.	22

Reference Books

Semester I

CHT 2201. Chemistry of Main Group Elements

1. Concise inorganic Chemistry, J.D. Lee, Wiley India
2. Inorganic Chemistry, P.W. Atkins
3. Advanced Inorganic Chemistry, Cotton and Wilkinson
4. Inorganic Chemistry: Principles of structure and reactivity: J. E. Huheey, E. A. Keiter, R. L. Keiter : Benjamin Cummings

CHT 2301. Organic Reaction Mechanism

1. Advance Organic Chemistry – Jerry March, Wiley-Interscience Publication
2. Organic Reaction Mechanism: M. G. Gallego, M. A. Sierra: Springer, Berlin
3. Modern Organic Reaction Mechanism: G. Whitmore: Sarup and Sons Publishers and distributers
4. Advanced Organic Chemistry: Part A and B: Francis Carey
5. Advance Organic chemistry, Reinhard Bruckner, Elsevier

CHT 2302. Heterocyclic chemistry

1. Heterocyclic Chemistry, J.A. Joule and K. Mills, Blackwell Publishing
2. Heterocyclic Chemistry-II, R. R. Gupta, M.Kumar, V. Gupta, Springer (India) pvt.

CHT 2401 Kinetics and Phase Equilibrium

1. Chemical Kinetics – K.J.Laidler
2. Concepts of modern kinetics and catalysis – I.Chorkendroff and J.W.Niemantsverdriet, Wiley VCH
3. Principles of Chemical Kinetics- J.C.House, C.Brown (1997)
4. Physical Chemistry, Maron and Pruton
5. Physical Chemistry, P.W. Atkins

CHT 2101 Instrumental methods of analysis

1. Instumental methods of analysis: Hobart H. Willard, Lynne L. Merritt, John A. Dean, Frank A. Settle : CBS Publishers and Distributers
2. Instrumental Methods of Analysis, Ed Sivasankar, Oxford University Press
3. Instrumental Methods of Chemical Analysis Hardcover – Galen W. Ewing, Barnes & Noble

CHT 2501. Material and Energy Balance

1. Basics principles of Chem. Engg calculations, Himmelblau
2. Chemical Process Principles Vol 1, Houghen, Watson, Ragatz

Semester II

CHT 2402 Quantum Chemistry

1. Quantum Chemistry, I.N. Levine, fifth edition - Prentice Hall
2. Molecular Quantum Mechanics, Atkins and Friedman.
3. Valence- C.A. Coulson, ELBS.
4. Introduction to quantum mechanics- L.Pauling and E.B.Wilson Quantum Chemistry, Ira N. Lavine
5. Quantum Chemistry, J.P.Low, K.A. Peterson, 3rd Edn., Elsevier
6. Fundamentals of quantum chemistry- James E House- (second edition) – Elsevier academic Press
7. Modern quantum chemistry- Attila Szabo and Neil S Ostlund- Dover publications
8. Quantum Chemistry, *D. A. McQuarrie*, Viva Books, New Delhi (2003)
9. Physical Chemistry, *P. W. Atkins*, Sixth Edition, Oxford University Press, Oxford
10. Physical Chemistry, *G. M. Barrow*, Fifth Edition, Tata McGraw Hill, New Delhi

CHT 2202 Chemistry of Transition metals

1. Concise inorganic Chemistry, J.D. Lee, Wiley India
2. Inorganic Chemistry, P.W. Atkins
3. Advanced Inorganic Chemistry, Cotton and Wilkinson
4. Inorganic Chemistry: Principles of structure and reactivity: J. E. Huheey, E. A. Keiter, R. L. Keiter : Benjamin Cummings

CHT 2303. Stereochemistry of Organic Compouds

1. Stereochemistry of organic compounds: Ernest L. Eliel, Samuel H. Wilen : A Wiley-interscience Publication
2. Stereochemistry, conformation and mechanism, P.S. Kalsi, New Age International, 2005
3. Stereochemistry of Organic compounds- Principles and Applications, D. Nasipuri, New Age International
4. Stereochemistry of Carbon compounds, E.L. Eliel, Tata-MacGraw Hill Education.

CHT 2402 Advanced Thermodynamics and Electrochemistry

1. Elements of Statistical Thermodynamics- L.K.Nash, Addison Wesley

2. Statistical Thermodynamics – B.J.McCelland, Chapman Hall
3. Thermodynamics and Statistical Thermodynamics – F.W.Sears, G.L.Salinger, Narosa
4. Modern Electrochemistry- J.O.M.Bockris and A.K.N.Reddy- Volumes I and II
5. Electrolytic solutions- R.A. Robinson and R.H. Strokes
6. Electrochemistry in Non-aqueous solutions by K. Izutsu.
7. Electrochemistry by Wolf Vielstich, Carl H. Haman, Andrew Hamnett, Teresa Iwasita, 2007

CHT 2304 Radicals, Photochemistry and Pericyclic reactions

1. Frontier Orbitals and organic Chemical reaction: Ian Fleming
2. Advanced Organic Chemistry: Part A and B: Francis Carey
3. Organic photochemistry, Coxon, Oxford University Press
4. Introduction to Organic photochemistry, J.D. Coyle, Wiley

CHT 2502. Fundamentals of Fluid flow and Heat transfer

1. Unit Operations in Chemical Engineering, McCabe and Smith

Semester III

CHT 2304. Organic Synthesis

1. Organic synthesis Michael B. Smith : McGraw-Hill
2. Organic Chemistry Clayden, Greeves, Warren and Wothers :Oxford University Press
3. Principles of Organic Synthesis R.O.C. Norman; Blackie academic and Professional
4. Mechanism in organic chemistry: R.O.C. Norman; Blackie academic and Professional
5. Organic synthesis: The Disconnection Approach, S.G. Warren and P. Wyatt, John Wiley & Sons.

CHT 2203. Organometallic Chemistry

1. The organometallic chemistry of the transition metals, Robert H. Crabtree, John Wiley & Sons
2. Organometallic Chemistry of Transition elements: F. P. Pruchnik: Springer
3. Organometallic Chemistry : R. C. Mehrotra: New Age International
4. Organometallic Chemistry: G. S. Sodhi: Ane Books Pvt. Ltd.
5. Organometallic reagents in Organic Synthesis: Paul R. Jenkins: Oxford Science Publications

6. Organometallics 1: Complexes with transition Metal-Carbon Sigma-Bonds: Manfred Bochmann: Oxford Science Publications
7. Organometallics 2: Complexes with transition Metal-Carbon pi-Bonds: Manfred Bochmann: Oxford Science Publications

CHT 2204 Solid State Chemistry, Molecular Symmetry and Group Theory

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

CHT 2305. Advanced Spectroscopy

1. Spectroscopy, Pavia, L., Kriz, V., Cengage Learning India Pvt Ltd
2. Spectrometric Identification of Organic Compounds, Robert M. Silverstein, Francis X. Webster, Wiley
3. Organic Spectroscopy: William Kemp, Palgrave
4. Principles of NMR in one and Two Dimensions: R. R. Ernst, G. Bodenhausen, A. Wokaun: Oxford Science Publication

Semester IV

CHT 2404 Biochemistry

1. Biotransformations in Organic Chemistry: Kurt Faber: Springer
2. Principles of Biochemistry, Lehninger, 4th Edition
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