M.Sc (Chemistry) Revised Syllabus (2022)

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 **three** electives in semester IV.
(4) Through many assignments and presentations the students are expected to acquire excellent presentation and communication skills.
(5) There is a major research component under **Project**. The students will be given research topics at the end of semester III and will work under the allotted guides.
(6) The laboratory courses in semesters I to III are open ended and enquiry driven.
(7) There will be in-semester and end-semester assessments for theory heads. 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 mid-semester examination carrying 30% 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 50:50. 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.
(8) There are a few audit courses for the benefit of students.
(9) 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.

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.

SEMESTER I

Course No.	Title	h/ week	Credits	Marks
CHT 2018	Chemistry of Main Group Elements	4	4	100
CHT 2002	Organic Reaction Mechanism	4	4	100
CHT 2003	Heterocyclic Chemistry	4	4	100
CHT 2004	Chemical Dynamics	4	4	100
CHT 2005	Instrumental Methods of Analysis	4	4	100
CHP 2001	Physical Chemistry Laboratory – I	4	2	100
CHP 2002	Organic Chemistry Laboratory – I	4	2	100
			24	

SEMESTER II

Course No.	Title	h/ week	Credits	Marks
CHT 2006	Quantum Chemistry	4	4	100
CHT 2007	Chemistry of Transition Metals	4	4	100
CHT 2008	Stereochemistry of Organic Compounds	4	4	100
CHT 2009	Molecular Thermodynamics	4	4	100
CHT 2010	Radicals, photochemistry and pericyclic reactions	4	4	100
CHP 2003	Organic Chemistry Laboratory – II	4	2	100
CHP 2004	Inorganic Chemistry Laboratory	4	2	100
			24	

SEMESTER III

Course No.	Title	h/ week	Credits	Marks
CHT 2011	Organic Synthesis	4	4	100
CHT 2012	Organometallic Chemistry	4	4	100
CHT 2013	Industrial Chemistry	4	4	100
CHT 2014	Organic Spectroscopy	4	4	100
CHT 2015	Solid State Chemistry and Group Theory	4	4	100
CHP 2005	Physical Chemistry Laboratory – II	4	2	100
CHP 2006	Instrumentation Laboratory	4	2	100
			24	

SEMESTER IV

Course No.	Title	h/ week	Credits	Marks
CHT 2016	Biochemistry	4	4	100
CHT 2017	Catalysis	4	4	100
CHT XXXX	Elective Paper I	4	4	100
CHT XXXX	Elective Paper II	4	4	100
CHT XXXX	Elective Paper III	4	4	100
CHP 2601	Project		8	**200**
			28	

Total Credits: 100, Total Marks: 2800

Elective Papers

CHT 2021	Natural Products
CHT 2022	Polymer Chemistry
CHT 2023	Surface and Interfacial Chemistry
CHT 2024	Computational Chemistry
CHT 2025	Nuclear Chemistry
CHT 2026	Bioinorganic Chemistry
CHT 2027	Developments in Organic Synthesis
CHT 2028	Supramolecular Chemistry
CHT 2029	Materials Chemistry
CHT 2030	Separation Processes
CHT 2031	Green Chemistry
CHT 2032	Material and Energy Balance

SEMESTER I

CHT 2018. Chemistry of Main Group Elements

Unit	Content	h
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), dπ- pπ 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/ Reference Books

1. J.D. Lee, *Concise Inorganic Chemistry*; 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 2002. Organic Reaction Mechanism

Unit	Content	h
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_N1, S_N2, S_Ni and S_N2' reactions. Reactivity: The effect of substrate structure, attacking nucleophile, leaving group, and reaction medium. Phase transfer catalysis, Ambient nucleophiles: Regioselectivity. Competition between S_N1 and S_N2 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: pKa 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/ Reference Books

1. Organic Chemistry–by J. Clayden, N. Greeves, S. Warren and P. Wothers (Oxford)
2. Advanced Organic Chemistry –by J. March 6th Edition
3. Advanced Organic Chemistry: Part A and B: Francis Carey
4. Advance Organic chemistry, Reinhard Bruckner, Elsevier
5. A guidebook to mechanism in organic chemistry – Peter Sykes 6th Ed.
6. Organic reaction mechanism (Benjamin) R. Breslow
7. Organic chemistry- R. T. Morrison and R. N. Boyd,(Prentice Hall.)
8. Organic Chemistry Vol. I (Sixth Edn.) and Vol. II (Fifth Ed.,) by IL Finar ELBS.
9. Mechanism and structure in Organic Chemistry – E. S. Gould
10. Modern Organic Reaction Mechanism: G. Whitmore: Sarup and Sons Publishers and distributers

CHT 2003. Heterocyclic Chemistry

Unit	Content	h
1	Introduction to heterocyclic chemistry, occurrence in nature and daily life applications such as drugs, dyes, optical brightners, natural products.	**4**
2	Nomenclature: Nomenclature of heterocyclic compounds. Trivial, Hantzch-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, Hanztsch 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, Hanztsch 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/ Reference Books

1. Heterocyclic Chemistry, J. A. Joules & K. Mills, Wiley-Blackwell publishing, 5th Edition
2. The Chemistry of Heterocycles: Structures, Reactions, Syntheses and Applications, Wiley-VCH, 2nd Edition
3. Heterocyclic Chemistry-II, R. R. Gupta, M.Kumar, V. Gupta, Springer (India)

CHT 2004 Chemical Dynamics

Unit	Content	h
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-ste p 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/ Reference Books

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

CHT 2005 Instrumental Methods of Analysis

Unit	Content	h
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 ad 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 dispersive devices, Energy dispersive devices, detectors, readout device, sample analysis using XRD	**6**

List of Text Books/ Reference Books

1. Skoog, Holler, Crouch, West - Fundamentals of Analytical Chemistry
2. David Harvey-Modern Analytical Chemistry
3. Quantitative Analysis, sixth edition- R.A. Day, A. L. Underwood
4. Pollard S.J.T., Thompson F. E., McConnachie G.L.-Ion Exchange Chromatography (1995)
5. Basics Gas Chromatography, Harold M. McNair, James Miller
6. Basic Gas Chromatography Mass Spectrometry, Principles and Techniques, F.W. Karasekand R.E. Clement, Elsevier, (Elsevier Science B.V.) 1988
7. 7) Introduction to Instrumental Analysis by R. D. Broun, Mc Graw Hill (1987)
8. 8) Instrumental methods of chemical analysis by H. willard, L.Merrit, J.A. Dean and F.A. settle. Sixth edition CBS (1986)

Practicals:

CHP 2001 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 2002 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 2006. 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	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_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.	8
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	6

List of Text Books/ Reference Books

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

CHT 2007 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	**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 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.	**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 one electron transfer reactions, outer sphere type reactions, cross reactions, inner sphere type reactions. Reaction mechanism of racemization and isomerization reactions	**10**

List of Text Books/ Reference Books

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 2008. Stereochemistry of Organic Compounds

Unit	Content	
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	**10**
2	**Strain and strain energy,** polycyclic compounds	**6**
3	**Resolution methods:** Types of racemic mixtures, resolution of racemic mixtures	**4**
4	**Conformational analysis:** Acyclic and cyclic compounds. Decalin	**8**
5	**Topocity and prostereoisomerism:** Homotopic ligands and faces, enantiotopic ligands and faces, diastereotopic ligands and faces.	**8**
6	**Stereoselective synthesis:** Additions, elimination, dihydroxylation, addition to carbonyl group – Felkin-Anh model,	**8**
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	**16**

List of Text Books/ Reference Books

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 2009. Molecular Thermodynamics

Unit	Content	h
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 form 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 transitions, lambda transitions- first order and second order phase transitions	**5**
10	Electrochemical equilibria – Electrochemical potentials, Poisson-Boltzmann model for distribution of electrolytes, Debye-Huckel theory Solvent interactions, heats of hydration, hydration number, pair formation, Bjrreum 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/ Reference Books

1. Physical Chemistry, P.W. Atkins
2. Elements of Statistical Thermodynamics- L.K.Nash, Addison Wesley
3. Statistical Thermodynamics – B.J.McCelland, Chapman Hall
4. Thermodynamics and Statistical Thermodynamics – F.W.Sears, G.L.Salinger, Narosa
5. Modern Electrochemistry- J.O.M.Bockris and A.K.N.Reddy- Volumes I and II

CHT 2010. Radicals, Photochemistry and Pericyclic Reactions

Unit	Content	h
	Radicals:	
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: SNAr reactions. Hoffman-Loffler-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, adamantine, 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/ Reference Books

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

Practicals:

CHP 2003 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 2004 Inorganic Chemistry Laboratory

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.

Semester III

CHT 2011. Organic Synthesis

Unit	Content	h
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, SmI_2, SeO_2 Corey-Chaykowsky reagent, DABCO, Gilmans 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 rearragentment, 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/ Reference Books

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

CHT 2012. Organometallic Chemistry

Unit	Content	h
1	History of Organometallic Chemistry: Nobel prizes awarded to this field and applications	**4**
2	Basic concept: Werner complexes, trans effect, Soft versus Hard ligands, Back bonding, Electroneutrality, Types of ligand	**6**
3	General Properties of Organometallic Complexes: 18- electron rule and its limitation, Electron counting in reactions, Bridged complexes, Metal-metal bond. Associative-Dissociative mechanisms	**6**
4	Classification of reactions: Oxidative addition, reductive elimination, insertion, β-Hydride elimination, σ-Bond metathesis, π-Bond metathesis	**6**
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**
6	Reactions of Metal-alkylss, metal-alkenes and metal-alkynes: Tsuji-Trost allylic alkylation, Reppe reaction, Pauson and Khand reaction	**6**
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	**6**
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	**6**
8	Bio-organometallic Chemistry: Basic concept of metals in biology having metal-carbon bond, cyanocobalamin, carboxyhaemoglobin, carbon monoxide dehydrogenase	**6**
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 CO2, CH.	**6**
10	Organometallic chemistry for meeting future challenges: Environment remediation for CO_2 utilization and depolymerization	**6**
11	Physical Methods in Organometallic Chemistry: Isolation procedures, 1H, 13C and 31P NMR, Dynamic NMR, Spin saturation transfer, IR Spectroscopy, Crystallography, Other methods	**4**

List of Text Books/ Reference Books

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

CHT 2013. Industrial Chemistry

Unit	Contents	h
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/ Reference Books

1. Industrial Organic Chemistry, 3rd, Completely Revised Edition, Klaus Weissermel, Hans-Jürgen Arpe ISBN: 978-3-527-61459-2 July 2008

2. 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.

3. Inorganic Chemistry – an industrial and environmental perspective, T.W. Swaddle, ISBN 0-12- 678550-3 , 482 pages, Academic Press

CHT 2014 Organic Spectroscopy

	Course Contents (Topics and subtopics)	h
	UV-Vis Spectroscopy:	
1	Electronic transitions, Chromophores, Auxochromes, Bathochromic and hypsochromic shifts, Solvent effects, Measurement of transmittance and absorbance, Beer Lambert's Law.	**4**
2	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.	**6**
	Vibrational Spectroscopy:	
3	Vibrational transitions, Selection rule, Modes of stretching and bending, FT-IR spectrophotometer.	**4**
4	Group frequencies, Factors affecting IR group frequency, NIR spectroscopy, Applications of vibrational spectroscopy in structural elucidation of organic compounds.	**8**
	^{1}H NMR Spectroscopy:	
5	Recapitulation of basic principle, Nuclear spin states and magnetic moments, Chemical shifts, Factors affecting the chemical shift, Shielding mechanism and anisotropic effects.	**5**
6	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	**7**
7	Nuclear Overhauser effect, Pulse technique, Solid state NMR, Interpretation of spectra and simplification of complex spectra.	**9**
	^{13}C NMR Spectroscopy:	
8	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.	**7**
	Mass Spectrometry:	
9	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.	**10**

List of Text Books/ Reference Books

1. Introduction to Spectroscopy, D.L. Pavia, G.M. Lampman, G.S. Kriz, J.R. Vyvyan, 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

CHT 2015 Solid state Chemistry and Group Theory

Unit	Content	h
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- Brillioun zones, k – space, Fermi surfaces and density states	**4**
	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	**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**

List of Text Books/ Reference Books

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.

Practicals:

CHP 2005 Physical Chemistry Laboratory II

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

CHP 2006 Instrumentation Laboratory

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

SEMESTER IV

CHT 2016. 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.	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/ Reference Books

1. Biotransformations in Organic Chemistry: Kurt Faber: Springer
2. Principles of Biochemistry, Lehninger, 4th Edition
3. Biochemistry, Voet andf Voet, 3rd Edition.
4. Biochemistry, Garret and Griesham
5. Bioorganic Chemistry, Dugas, H, Springer
6. Bioorganic Chemistry – Carbohydrates and Nucleic acids, Hecht (editor)
7. Bioorganic Chemistry, Soni, R.K. and Sharma, P, Saujanya Book, 2008

CHT 2017. Catalysis

Unit	Content	h
1	**Types of catalysis:** Heterogeneous and Homogeneous catalysis. Catalytic cycles. TON, TOF	**4**
	Catalyst preparation: Bulk and supported catalysts, deactivation and regeneration.	**6**
	Characterization of catalysts: Surface area, surface acidity and basicity, XPS, UPS, AES, EXAFS, XANES, XRD TPD.	**10**
2	**Heterogeneous catalysis:** Adsorption isotherms, kinetics of heterogeneous catalytic reactions, structure of adsorbed species.	**8**
	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.	**8**
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,	**12**
5	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	**12**

List of Text Books/ Reference Books

1. Catalysis from principles to applications, Eds. Matthias Beller, Albert Renken and Rutger A. van Santen, Wiley-VCH
2. Principles and practice of heterogeneous catalysis - J.M.Thomas and W.J.Thomas-VCH publications, NY
3. Catalysis- concepts and green applications- Gadi Rothenberg-Wiley VCH
4. Homogeneous catalysis- mechanism and industrial applications- S.Bhaudri and D.Mukesh, John Wiley and sons
5. Design of heterogeneous catalysts –U.S.Ozkan (ed) – Wiley VCH
6. Introduction to surface chemistry and catalysis- G.A. Somarjai, Wiley and sons.
7. Heterogeneous catalysis, D.K. CHakrabarty and B. Viswanathan, New Age Publishers, New Delhi

Elective Paper I CHT XXXX

Elective Paper II CHT XXXX

Elective Paper III CHT XXXX

CHP 2007 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.

ELECTIVE PAPERS

CHT 2021. Natural Products

Unit	Content	h
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, occurance, 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 pyrenthrin, chrysanthemic acid, metofluthrin.	**6**

List of Text Books/ Reference Books

1. Chemistry of Natural Product: Sujata V. Bhat, Bhimsen A. Nagasampagi, M. Sivakumar: Springer.
2. Organic Chemistry of Natural Products, G. R. Chatwal: Himalaya Publications, New Delhi
3. Organic Chemistry, Vol II, I. L. Finar , ELBS
4. Terpenoids: V. K. Ahluwalia: Ane Books Pvt. Ltd.
5. Steroids and Hormones: V. K. Ahluwalia: Ane Books Pvt. Ltd.
6. Antibiotics : V. K. Ahluwalia: Ane Books Pvt. Ltd.

CHT 2022. Polymer Chemistry

Unit	Content	h
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:** Viscocity, 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/ Reference Books

1. Polymer Science: V. R. Gowariker, N.V.Vishwanathan, Jayadev Sreedhar New Age International (P) Limited, Publisher.
2. Polymers: David Walton and Phillip Lorimer: Oxford Science publications
3. Polymer Science: V. K. Ahluwalia, Anuradha Mishra: Ane Books pvt. Ltd.

CHT 2023. Surface and Interfacial Chemistry

Unit	Content	h
1	Concept of surface free energy and surface tension, interfacial tension and interfacial free energy, surface excess.	**6**
2	**Liquid surfaces**	
	2.1 Thermodynamics of liquid surfaces: Gibbs adsorption isotherm, spreading coefficient and wetting phenomena.	**8**
	2.2 Thermodynamics of curved surfaces: Young, Laplace, Kelvin, and Thomson equations.	**6**
	2.4 Potentials of interfaces, interfacial viscosity. Insoluble monolayers, LB films and molecular self assembly.	**8**
	2.4 Bubbles and foams, homogeneous and heterogeneous nucleation.	**6**
3	**Solid- liquid interfaces:** Work of adhesion and cohesion, wetting and contact angles, adsorption from solution at solid/ liquid interfaces, critical surface tension.	**6**
4	**Surfactants** Introduction: General structure, types, nomenclature Surfactant aggregates – Factors affecting aggregational behaviour	**6**
	Synthesis of surfactants: Synthesis of hydrophobes, functionalisation of hydrophobes	**4**
	Applications of surfactants, Biosurfactants and biodegradable surfactants, Mixed surfactant systems	**4**
5	Emulsions, microemulsions, gels, foams, colloids.	**4**
6	Hydrotropes: Nature, structure, behavior, applications	**2**

List of Text Books/ Reference Books

1. An introduction to the principles of surface chemistry- Aveyard
2. Micelles- Theoretical and applied aspects- Y.Morai
3. Surface activity- principles and applications- Kaoru Tsujii
4. Fundamentals of colloid science- Robert J Hunter- Vol I and II
5. Colloid chemistry- Shaw
6. Surfaces, interfaces and colloids, Meyers
7. Physical Chemistry of surfaces, Adamson
8. Surfactant Systems: their chemistry, pharmacy and Biology by D. Attwood and A.T. Florence-London, Chapman and Hall 1983.
9. Surfactant and Interfacial phenomena by M.J. Rosen, 2nd Edition, Wiley interscience publications 1989
10. Surfactants: Chemistry and properties by Anthony J O'Lenickllinois: Allured publication 1999

CHT 2024. Computational Chemistry

Unit	Content	h
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/ Reference Books

1. Computational Chemistry, A.C. Norris, John Wiley.
2. Computer Programming in FORTRAN 77, R. Rajaraman, Prentice Hall.
3. Essentials of Computational Chemistry, 2nd Edn., C.J.Cramer, Wiley
4. The basis of theoretical and computational Chemistry, B.M.Rode, T.S. Hofer, Wiley VCH
5. Numerical Analysis, C.E. Frogberg, Macmillan.
6. Numerical Analysis-A Practical Approach, M.J.Maron, John Wiley.
7. Numerical Methods for Scientists Engineers, H.M. Antia, Tata McGraw Hill.

CHT 2025. 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	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/ Reference Books

1. Principles of Radiochemistry, Eds-Sood, Ramamoorthy & Reddy (IANCAS, BARC, Mumbai)
2. Radiation Chemistry: An Overview-D. B. Naik and S. Dhanya (BARC, Mumbai)
3. Nuclear and Radiation Chemistry-Friedlander, Kennedy Macias & Miller (Wiley) 1981
4. Essentials of Nuclear Chemistry- H.J.Arnikar (Wiley Eastern) 1987.
5. An Introduction to Radiation Chemistry-Spinks and Woods (Wiley, New York) 1990.
6. Nuclear Chemistry; New Jersey, Prentice Hall Inc., 1965.
7. Nuclear Chemistry by N.R. Johnson, E. Eichler & G. D. O Kelley-New York John Wiley & Sons. 1963.
8. Nuclear Chemistry and its applications- M. Haissinsky and D.G. Tuck

CHT 2026 Bioinorganic Chemistry

Unit	Content	
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	Biomineralization	**2**

List of Text Books/ Reference Books

1. S. J. Lippard and J. M. Berg, Principles of bioinorganic chemistry, University Science Books, Mill Valley, 1994.
2. I. Bertini, H. B. Gray, S. J. Lippard and J. S. Valentime, Bioinorganic Chemistry, Univ. Sci. Books, Mill Valley, 1994.
3. J. A Cowan, Inorganic Biochemistry, VCH Publishers, 1993.
4. R. W. Hay, Bioinorganic Chemistry, Ellis Hollwood, Ltd.1984.
5. W. Kaim and B. Schwederski, Bioinorganic Chemistry: Inorganic elements in the chemistry of life (An introduction and guide), John Wiley & Sons

CHT 2027. Developments in Organic Synthesis

Unit	Content	h
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/ Reference Books

1. Alternate Energy Processes in Chemical Synthesis: Microwave, Ultrasonic and Photo Activation By, V K Ahluwalia, Rajender S Varma
2. Organic Synthesis Engineering(Hardcover - 2001-02-15) by L. K. Doraiswamy
3. Ionic Liquids in Organic Synthesis Edited by Sanjay V. Malhotra
4. Green Solvents, Volume 6: Ionic Liquids. Paul T. Anastas, ISBN: 978-3-527-325924
5. Visible-Light-Active Photocatalysis: Nanostructured Catalyst Design Mechanisms And Applications by Srabanti Ghosh, John Wiley, ISBN: 9783527342938
6. Solid-Supported Catalysis, https://doi.org/10.1002/9781119288152.ch11
7. Activation of Small Molecules: Organometallic and Bioinorganic Perspectives, ISBN: 9783527609352
8. Related review articles.

CHT 2028 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.	**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/ Reference Books

1. J.-M. Lehn; Supramolecular Chemistry-Concepts and Perspectives (Wiley-VCH, 1995)
2. P. D. Beer, P. A. Gale, D. K. Smith; Supramolecular Chemistry (Oxford University Press, 1999).
3. J. W. Steed and J. L. Atwood; Supramolecular Chemistry (Wiley, 2000)

CHT 2029. 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.	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
14	**Applications of nanoparticles:** industry, medical field, research. Environmental issue. Toxicity and biosafety in application of nanoparticles	6

List of Text Books/ Reference Books

1. Introduction to materials chemistry, Harry R. Allcock, John Wiley and Sons Inc, New York.
2. Introduction to Solids, Leonid V. Azaroff, Tata McGraw-Hill Publishing Company Ltd
3. Introduction to the Physics and Chemistry of Materials, Robert J. Naumann: Boca Raton: CRC Press
4. Material Chemistry: Bradley D. Fahlman: Springer-Verlag, New York
5. Materials Chemistry, Fahlman B.D., Springer
6. Nanomaterials and Nanochemistry, Br'echignac C., Houdy., and Lahmani M. (Eds.)Springer Berlin Heidelberg New York. 2007.
7. Nanoparticle Technology Handbook. M. Hosokawa, K. Nogi, M. Naito and T Yokoyama (Eds.) First edition 2007. Elsevier
8. Nanotechnology Basic Calculations for Engineers and Scientists. Louis Theodore, John Wiley & Sons Inc., 2006

CHT 2030 Separation Processes

Unit	Content	h
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/ Reference Books

1. Unit Operations in Chemical Engineering, McCabe and Smith

CHT 2031 Green Chemistry

Unit	Content	h
	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/ Reference Books

1. Green Chemistry. Theory and Practice. Paul T. Anastas and John C. Warner.
2. Green Chemistry: An Introductory Text: Edition 3 – Mike Lancaster
3. Introduction To Green Chemistry by Albert S. Matlack

CHT 2032. Material and Energy Balance

Unit	Content	h
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/ Reference Books

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