

# **INSTITUTE OF CHEMICAL TECHNOLOGY**

## **Department of Chemistry**

(Recognized by University Grants Commission for SAP-DRS-1 programme)

### **Rules and Regulations of Syllabi relating to the Degree of Master of Science in Chemistry (M. Sc. Chemistry)**

#### **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. Particular mention should be made of developments in biological sciences at the molecular level, which need deep understanding of Chemistry. Developments in materials science are also mainly from chemistry side. Due to these developments the traditional M.Sc. Chemistry courses may not be very effective and meaningful in the present age.

It is observed that if the Chemistry students know basic principles of Chemical Engineering, they are more effective at the application level. The bridge courses offered in some of the foreign universities, which are offered to nonchemical engineering students before they take up formal chemical engineering, are found to be useful in this context.

On this background it is felt that a new course of Chemistry is needed at the post-graduate level, which will essentially be of our interdisciplinary nature. The course should not be compartmentalized as Inorganic Chemistry, Organic Chemistry, Physical Chemistry, etc. but should be a modular course, with relevant units. Some of these units will cut across the traditional branches of chemistry. The present course has been framed with these objectives. The Institute of Chemical Technology has a unique advantage of having expertise in Chemical Engineering and Chemical Technology. Thus, this expertise will be available in-house.

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

### 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 who have taken 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 and mathematics as the two other subjects at the first and second years, of University of Mumbai or of any other recognized University; and passed the qualifying examination with at least 60% of the marks in aggregate or equivalent grade average. [55% for the backward class candidates only from Maharashtra State] are only eligible to apply.
- (b) The candidates shall have cleared the qualifying examination in one seating; i.e. repeaters shall not be eligible for the admission.
- (c) The admissions will be done strictly on the basis of merit, based on the marks obtained in the qualifying examination.

### 3. Course structure

- (a) The course is a credit-based 4-semester (2-year) course.
- (b) There will be two semesters in a year: July to December - semester I, and December to May - semester II. Each semester will consist of 15-16 weeks of instructions including seminars / projects/assignments.
- (c) At the end of each semester the candidates will be assessed as per the norms of the Institute.
- (d) Various activities associated with the semesters will be carried out as per the academic calendar of the Institute.
- (e) The requirement of attendance of the students shall be as per the norms of the Institute.
- (f) All the relevant academic regulations of the Institute shall be applicable to the course.
- (g) Assessment of the students will be done as per the norms of the Institute.
- (h) In case of any difficulty regarding any assessment component of the course, the Departmental Committee shall take appropriate decision, which will be final.
- (i) **Electives:** The electives to be offered during a given academic year will be decided by the Departmental Committee before the beginning of the year and will be announced by the Head. The students have to take electives from this list only.

(j) **Project:**

- (i) At the beginning of the Second semester, the Head of Department in consultation with the Departmental Committee will assign topics for the projects to the students and assign the supervisors.
- (ii) The students will also be required to do literature survey and submit the same to the respective supervisors before end of Semester III.
- (iii) The students will do the experimental work in the semester IV on the topics assigned.
- (iv) The students shall submit the project report before the prescribed date which will be a date before the last date of the semester IV. The report shall be submitted with soft binding.
- (v) The project report will be examined by the supervisor along with one other internal/external referee to be appointed by the Departmental committee. The referees shall give marks to the report as per the norms.
- (vi) The students will make presentation on the work in front of the Project Evaluation Committee (PEC) appointed by the Departmental Committee, in open defense form. The PEC will give marks to the presentation.
- (vii) The comments received from the referees as well as given by the PEC need to be incorporated in the thesis in consultation with the supervisor, before doing the hard binding. The thesis in the hard copy form will be maintained in Department office.
- (viii) Final copy of the thesis will be submitted to the Institute in hard-bound form.

#### 4. Semester wise pattern of the M.Sc. – Chemistry course.

##### SEMESTER I

Course No.	Title	h/week	Credits	Marks
CHT 2301	Chemistry of Main Group Elements	2 + 1T	3	50
CHT 2401	Organic Reaction Mechanism	2 + 1T	3	50
CHT 2501	Thermodynamics and Phase Equilibrium	2 + 1T	3	50
CHT 2201	Material and Energy Balance	2 + 1T	3	50
CHT 2302	Materials Chemistry	2 + 1T	3	50
CHT 2XXX	Elective Paper I	2 + 1T	3	50
				300
CHP 2301	Inorganic Chemistry Laboratory	4	2	50
CHP 2501	Physical Chemistry Laboratory-I	4	2	50
CHP 2401	Organic Chemistry Laboratory-I	4	2	50
				150
			24	450

## SEMESTER II

Course No.	Title	h/week	Credits	Marks
CHT 2303	Chemistry of Transition metals	2 + 1T	3	50
CHT 2402	Stereochemistry	2 + 1T	3	50
CHT 2502	Chemical Reaction Kinetics	2 + 1T	3	50
CHT 2101	Instrumental Methods of Analysis	2 + 1T	3	50
CHT 2202	Fundamentals of Fluid Flow and Heat Transfer	2 + 1T	3	50
CHT 2XXX	Elective Paper II	2 + 1T	3	50
				300
CHP 2201	Chemical Engineering Laboratory	4	2	50
CHP 2502	Physical Chemistry Laboratory-II	4	2	50
CHP 2402	Organic Chemistry Laboratory-II	4	2	50
				150
			24	450

## SEMESTER III

Course No.	Title	h/week	Credits	Marks
CHT 2403	Organic Synthesis	2 + 1T	3	50
CHT 2102	Advanced Spectroscopy	2 + 1T	3	50
CHT 2304	Organometallic Chemistry	2 + 1T	3	50
CHT 2503	Molecular Spectroscopy and Bonding	2 + 1T	3	50
CHT 2103	Separation Chemistry	2 + 1T	3	50
CHT 2XXX	Elective Paper III	2 + 1T	3	50
				300
CHP 2503	Physical Chemistry Laboratory-III	4	2	50
CHP 2403	Organic Chemistry Laboratory-III	4	2	50
CHP 2101	Analytical Chemistry Laboratory	4	2	50
				150
			24	450

## SEMESTER IV

Course No.	Title	h/week	Credits	Marks
CHT 2404	Bioorganic Chemistry	2 + 1T	3	50
CHT 2XXX	Elective Paper IV	2 + 1T	3	50
CHT 2XXX	Elective Paper V	2 + 1T	3	50
CHT 2XXX	Elective Paper VI	2 + 1T	3	50
CHT 2701	Chemical Project Economics	2 + 1T	3	50
CHP 2001	Seminar	2 + 1T	3	50
				300
CHP 2002	Project		6	150
				150
			24	450

**Total Credits: 96, Total Marks: 1800**

### Elective Papers

- CHT 2511. Catalysis
- CHT 2512. Industrial Engineering Chemistry
- CHT 2411. Natural Products
- CHT 2412. Polymer Chemistry
- CHT 2413. Heterocyclic chemistry
- CHT 2414. Radicals, Photochemistry and Pericyclic Reactions
- CHT 2513. Surface and Interfacial Chemistry
- CHT 2415. Developments in Organic Synthesis
- CHT 2611. Green Chemistry
- CHT 2514. Quantum Chemistry
- CHT 2416. Unit Processes in Organic Synthesis
- CHT 2417. Pharmaceuticals Chemistry
- CHT 2418. Pesticides
- CHT 2515. Electrochemistry
- CHT 2419. Chemistry of Oleochemicals
- CHT 2516. Chemistry of Surfactants
- CHE2517. Computational Chemistry
- CHE2311. Nuclear Chemistry
- CHE2420. Chemistry of colorants

## C. Detailed Syllabus of the M.Sc. –Chemistry Course

### SEMESTER I

#### CHT 2301. Chemistry of Main Group Elements

- 1. s-block elements:** Comparative study and diagonal relationship. Salient features of hydrides, salvation and complexation tendencies, function in biosynthesis. **4**
- 2. p-block elements:** Comparative study (including diagonal relationship) of Group 13-17 elements. Hydrides, oxides, oxyacids, and halides, hydrides of boron - diborane and higher boranes, borazine, borohydrides, fullerenes, carbides, fluorocarbons, silicates (structural principles), tetrasulfur tenitride. Basic properties of halogens. Interhalogens and polyhalides. **6**
- 3. Stereochemistry and bonding in main group elements:** VSEPR, Walsh diagrams (tri- and penta- atomic molecules),  $d\pi-p\pi$  bonds, Bent rule and energies of hybridization. Simple reactions of covalently bonded molecules. **3**
- 4. Noble gases:** Chemical properties of noble gases, chemistry of xenon, structure and bonding in xenon compounds. **3**
- 5. Lanthanides:** Occurrence and isolation. Electronic structure, oxidation states. Lanthanide contraction and ionic radii. Lanthanide compounds and complex formation, **4**
- 6. Actinides:** General features and chemistry of actinides, chemistry of separation of Np, Pu and Am from U. Similarities between later actinides and later lanthanides. **4**
- 7. Silicones and Phosphazenes:** Silicones and phosphazenes as examples of inorganic polymers, nature of bond in triphosphazines. **2**
- 8. Metal clusters:** Higher boranes, carboranes, metalloboranes and metallocarboranes, metal carbonyls and halide clusters, compounds with metal-metal multiple bonds. **4**

#### CHT 2401. Organic Reaction Mechanism

- 1. Methods of determining reaction mechanism:** Trapping of intermediates. Cross over experiments, isotopic effect and labeling, stereochemical studies, kinetic effect, Salt effect, Energy profile diagram. Concept of transition state and reaction coordinate. FMO theory and its applications. Acid-Base concepts. Solvent effects **6**
- 2. Substitution:**  $S_N1$ ,  $S_N2$ ,  $S_Ni$ ,  $S_NCA$  reactions, NGP **4**
- 3. Elimination:**  $E_1$ ,  $E_2$ ,  $E_{1cB}$ , Zaitsev and Hoffmann elimination **3**
- 4. Addition reaction:** Hydroxylation and dihydroxylation of olefins  
Esterification and hydrolysis of esters **2**
- 5. Chemistry of enolate ions:** Generation and reactions. Thermodynamic and kinetic control **5**
- 6. Neutral high energy intermediates:** Ketenes, carbenes, nitrenes, singlet oxygen: Their Generation, structure and reactions  
Tautomerism including ring-chain and valence tautomerism **6**

**7. Aromaticity:** Criteria of aromaticity. Huckel MO theory, Frost-Muslin geometrical interpretation. Application to carbocyclic and heterocyclic systems, ferrocenes, azulenes, annulenes, tropylium ion, fulvenes, sydnones. Recent ideas of aromaticity **4**

## **CHT 2501 Thermodynamics and Phase Equilibrium**

### **1. Equilibrium Thermodynamics**

1.1 Brief review of laws of thermodynamics and thermodynamic functions, chemical equilibrium- chemical potential and partial molar properties, Gibbs Duhem equation, vant Hoff isochor and isotherm.

Heats of formation and Reaction, effect of temperature on Heats of reaction and equilibria **6**

1.2 Nernst heat theorem, third law of thermodynamics, entropy and probability, and entropy of mixing. **4**

1.3 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. **4**

### **2. Non-equilibrium Thermodynamics**

2.1 Thermodynamics of irreversible processes, conversion of mass and energy in open and closed systems, non adiabatic processes, generalized forces and fluxes, Clausius inequality **4**

2.3 Nonequilibrium thermodynamics: Postulates and methodologies, linear laws. **2**

### **3. Molecular Thermodynamics**

3.1 Concepts of micro states and micro configuration, degeneracy. **4**

3.2 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 **6**

## **CHT 2201. Material and Energy Balance**

1. Units and Dimensions. Mole concept. Compositions relationship. **4**

2. Reaction stoichiometry. **3**

3. Behaviour of gases and vapours. Humidity and vaporization. **5**

4. Simple material balance without reaction. **4**

5. Material balance with chemical reaction. Complex material balance. **4**

6. Energy balance associated with reactions. **4**

7. Simultaneous material and energy balance. Combustion calculation. **4**

8. Atom economy **2**

## CHT 2302. Materials Chemistry

1. **Alloys:** Ferrous and Nonferrous alloys. 3
2. **Metals:** metal clusters, bonding in solids- metals, semiconductors, imperfections in solids. Amorphous solids 3
3. **Glasses & Ceramics:** Glassy state, glass formers and glass modifiers. Ceramic structure. Mechanical properties. 3
4. **Clays and refractory materials:** Classification, structure and modifications of clays. Properties and applications of clays. **Refractories:** Classification, properties and applications. Microscopic composites. 3
5. **Dyes:** Chromophore structure. Synthesis of typical dyes. Chemiluminescence. Photochromics. Colour photography. 3
6. **Liquid crystals:** Classification, thermotropic/lyotropic, calamitic/discotic, nematic/smectic/columnar. Synthesis, orientation, LC displays. LC polymers 2
7. **Thin Films and LB films:** Preparation and applications 2
8. **Electronic 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 4
9. **Fullerenes** 1
9. **Supramolecular chemistry:** Molecular complexes. Molecular recognition. Crown ethers, cryptands, cyclodextrins, calixarenes, cavitands. Supramolecular devices. Self assemblies. 3
10. **Ionic liquids** 1
11. **Polymers and composites** 2

### Practicals:

#### CHP 2301 Inorganic Chemistry Laboratory-I

Preparation and characterization of inorganic complexes containing Fe, Co, Ni, Cu, Zn, with N, and P containing ligands. Applications of these complexes for Organic coupling reactions like Heck, Suzuki, Stille and Sonogashira reactions.

#### CHP 2502 Physical Chemistry Laboratory-I

Determination of thermodynamic parameters and partial molar volume, determination of interaction parameters from distribution coefficients and equilibrium constants, determination of iso electric points, experiments based on phase equilibrium.

#### CHP-2401 Organic Chemistry Laboratory-I

Separation and purification techniques – Extraction, crystallization, distillation chromatography.



## SEMESTER II

### **CHT 2303. Chemistry of Transition Metals**

- 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. **4**
- 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. **4**
- 3. Electronic spectra of transition metal complexes:** Types of electronic transition, selection rules for d-d transitions, spectroscopic ground states, spectrochemical series, Orgela and Tanabe-Sugano diagrams for transition metal complexes ( $d^1$ - $d^9$  states), calculations of Dq, B and beta parameters, charge transfer spectra, discussion of the electronic spectrum of  $[\text{Ti}(\text{H}_2\text{O})_6]^{3+}$  complex ion. **3**
- 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. **3**
- 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. **5**
- 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. **4**

## CHT 2402. Stereochemistry

- 1. Stereochemistry of** – (i) compounds with two or more stereocentres. (ii) 3,4,5 membered ring compounds (iii) 6-membered ring compounds (iv) fused ring compounds – decalins. (v) molecules with tricoordinate and tetracoordinate centres – N, S, Si, P, As. (vi) allenes, spiranes, biphenyls, ansa compounds, cyclophanes **12**
- 2. Resolution methods:** Types of racemic mixtures, resolution of racemic mixtures **3**
- 3. Topocity and prostereoisomerism:** Homotopic ligands and faces, enantiotopic ligands and faces, diastereotopic ligands and faces. **2**
- 4. 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. **13**

## CHT 2502 Chemical Reaction Kinetics

- 1. Reaction kinetics :** kinetics of simple reactions, temperature effect on reaction rate, steady state treatment, application of kinetic studies in elucidating reaction mechanism. Development of rate expressions, methods of determining parameters of rate expressions, Reactions in molecular beams, kinetics of photochemical reactions **15**
- 2. Mass Transfer:** Mass transfer effects on reaction kinetics and processes. Agitation and mixing of liquids **5**
- 3 Homogeneous Reactions:** Kinetics of homogeneous acid base reactions, auto catalytic and oscillatory reactions, kinetics of fast reactions. **5**
- 4. Heterogeneous Reactions,** surface reactions; identification of rate determining steps **5**

## CHT 2101. Instrumental Methods of Analysis

- 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 **4**
- 2. Instruments:** pH meter, refractometer, conductometer, polarimeter – basic principles critical parameters affecting them, use, merits and demerits. Instrument calibration and validation. Certified reference materials. Maintenance and trouble shooting. **5**
- 3. Flame spectrometry:** FES, AAS, AFS **1**
- 4. Molecular Luminescence:** Fluorescence, Phosphorescence, Chemical/Bio Luminescence **1**
- 5. Aquametry:** Karl-Fischer, moisture in gases **1**

<b>6. Electroanalytical method:</b> Conductometry, potentiometry, voltmetry, cyclic voltmetry, coulometry, ion selective electrodes and sensors, polarography, anodic/cathodic stripping,	<b>5</b>
<b>7. Diffraction techniques:</b> Unit cells and Bravais lattices, Miller indices, Powder diffraction pattern, Neutron and X-ray diffraction methods.	<b>4</b>
<b>9. Thermoanalytical methods:</b> DTA, TGA, DSC	<b>3</b>
<b>10. Radio analytical methods:</b> Analytical applications of radioisotopes, neutron activation analysis, isotope dilution analysis.	<b>2</b>
<b>12. Surface Characterization:</b> SEM, TEM, AFM	<b>2</b>
<b>13. Scattering:</b> Turbidimetry, nephelometry, Raman spectroscopy.	<b>2</b>

## **CHT 2202. Fundamentals of Fluid Flow and Heat Transfer**

<b>1. Fluid characteristics:</b> Viscosity, density, pressure, surface tension. Newtonian and non-newtonian fluids.	<b>4</b>
<b>2. Types of flow:</b> Laminar and turbulent flow.	<b>3</b>
3. Flow characteristics, flow measurement,	<b>4</b>
4. Fluid passed immersed bodies. Flow through pipes. Mixing in fluids	<b>3</b>
5. Transportation and metering of fluids.	<b>3</b>
6. Agitation and mixing of liquids.	<b>3</b>
7. Heat transfer to fluids with and without phase change. Mechanism of Heat transfer: Conduction and convection.	<b>4</b>
8. Evaporation, boiling, refrigeration.	<b>3</b>
9. Heat exchangers, heat transfer media	<b>3</b>

### **Practicals:**

## **CHP 2201 Chemical Engineering Laboratory**

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).

Experiments to determine rate laws and rate constants, oscillatory and clock reactions, kinetic measurements through optical rotation measurements. Study of effect of ionic strength/ solvent on reaction kinetics. Catalytic effects on reactions

## **CHP 2502 Physical Chemistry Laboratory-II**

Conductometric and potentiometric titrations of multi component systems, determination of transport number, determination of solubility products, stability constants, thermodynamic data from emf measurements, experiments based on cyclic voltametry and polarography, experiments based on surface/interface chemistry and macromolecules

## CHP 2402 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. Estimations of functional groups.

## CHT 2403. Organic Synthesis

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. **Selectivities in synthesis:** Chemoselectivity, regioselectivity, stereoselectivity, atom selectivity. **1**
3. **Functional groups:** Their reactivity profile, interconversions and protection. Umpolung, **1**
4. **Ylides:** Ylides of P and S. Wittig reaction and its modifications, **1**
5. **Enamines:** Synthesis, reactivity and synthetic importance. **1**
6. **Ring cyclization methods:**
7. **Reduction:** Catalytic hydrogenation. Dissolving metal reductions. Hydride transfer reagents. Complex hydrides including nucleophilic, electrophilic and radical reducing agents. Organo boranes. MVP reduction. **3**
8. **Oxidation:** Cr, Os, Ti, Fe and Mn reagents, per acids and peroxides, Oxidation by ozone, oxygen, Swern oxidation. Bayer Viliger oxidation **3**
9. **Selected organic reagents:** TMSC/I, TBTH, DCC, DDQ, TCQ, CAN, NBS, DIBAL, PTC, Crown ethers, SmI<sub>2</sub>, SeO<sub>2</sub> **3**
10. **Selected name reactions:** Hoffmann-Löffler-Fritag reaction, Sharp reaction, Paterson reaction, Heck reaction, McMurry coupling reaction, Suzuki reaction, Birch reduction, Woodward-Prevost reaction, Chichibabin reaction, Mukaiyama esterification, Mitsunobu reaction. **4**
11. **Rearrangements:** Favorskii reaction, Curtius Lossen, Benzil-Benzilic acid rearrangement, Steven, Shapiro, Tiffenev-Demyanov, Benzidine rearrangement **3**
12. **Strained molecules:** Prismanes, cubane, and other strained molecules. Adamantane **1**
13. **Fascinating Organic synthesis:** Reserpine, Longifoline, Grisofulvin, Quinine, Oestrone, B-vetivone, Colchicine **3**  
New Energy sources **1**
14. **Nonconventional energy sources:** Microwaves and ultrasound based synthesis **1**

## CHT 2102. Advanced Spectroscopy

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. Raman spectroscopy. **3**

<b>3. NMR spectroscopy:</b> Basic theory. <b>H1 NMR:</b> Chemical shifts and factors affecting the same, spin-spin coupling of different systems. Simplification of complex spectra. Pulse technique. <b>C13 NMR:</b> Basics, double resonance. <b>F19 and P31 NMR.</b> <b>2D NMR.</b> NOE. Solid state NMR.	<b>7</b>
<b>4. Mass spectrometry:</b> Basics. Different techniques. Isotopic abundance. Fragmentation. Rearrangement of ions.	<b>5</b>
<b>5. Hyphenated techniques.</b>	<b>4</b>
<b>6. ESR spectroscopy:</b> Theory, experimental technique, Hyperfine splitting	<b>2</b>
<b>7. Mossbauer spectroscopy</b> Emission: Flame photometry, ICP, Ark-Spark spectra, Phosphorescence, XRF Structure elucidation using combined stereoscopic methods	<b>4</b>
<b>8. ESCA:</b> X-ray absorption and emission spectra	<b>2</b>

## CHT 2304. Organometallic Chemistry

<b>1. Nature of C-M bond:</b> Metal-carbon bond with main group and transition elements.	<b>1</b>
2. Factors controlling metal-carbon bond formation. Methods of M-C bond formation.	<b>1</b>
3. Nomenclature and hapticity. Electron counting and 16 and 18 electron rules - applications and exceptions. Stability. Stereochemical nonrigidity in organometallic compounds.	<b>2</b>
4. Structure and bonding of metal alkyls and aryls.	<b>2</b>
5. Complexes with CO and related ligands, olefins, acetylenes and related unsaturated molecules.	<b>3</b>
6. Organic transition metal complexes as protective and stabilizing groups for double bond, triple bond, propyl cation and short lives species.	<b>2</b>
7. Complexes with cyclopentadiene and arenes and other C <sub>n</sub> H <sub>n</sub> sandwich and half-sandwich complexes. Hydride, dinitrogen and dihydrogen complexes	<b>2</b>
<b>8. Bimetallic and cluster complexes:</b> Structure and applications in catalysis	<b>1</b>
<b>9. Basic organometallic reactions:</b> Ligand substitution, oxidative reactions, migratory reactions, migratory insertion, extrusion, oxidative addition, reductive elimination, reductive elimination –mechanism and stereochemistry.	<b>5</b>
<b>10. Nucleophilic reagents with C-M bond:</b> Li, Mg, Al, Ti and Ce alkyls; Organocuprates, organic zinc reagents	<b>4</b>
11. Alkyne complexes: Pauson Khand reaction.	<b>1</b>
12. The use of stoichiometric transition metal complexes in the synthesis of complexes organic molecules - enantioselective synthesis via organometallic compounds.	<b>3</b>
13. Organo silicon compounds, boranes, carboranes and, metallocarboranes, organo platinum complexes, metallocenes	<b>2</b>
14. Importance of organometallic compounds in Biological systems	<b>1</b>

## CHT 2503 Molecular Spectroscopy and Bonding

1. MO theory of diatomic molecules, Born-Oppenheimer approximation, H<sub>2</sub> molecule, correlation diagrams. 4
2. Valence bond theory of simple molecules, hybridization, comparison of VB and MO theories. 3
3. MO diagrams of simple triatomic molecules, pi electron systems, Huckel treatment for conjugated hydrocarbons, electron density and bond order. 4
4. **Molecular spectroscopy:**
  - 4.1 Electromagnetic radiations, spectral line width, selection rules, Fourier Transformation and computer averaging, width and intensity of spectral lines 2
  - 4.2 **Rotational spectroscopy:** classification of molecules based on moment of inertia, non rigid rotor, linear triatomic molecules, symmetric top molecules, Stark effect. 3
  - 4.3 **IR Spectroscopy:** IR spectra of diatomic molecules, selection rule, unharmonicity, Morse potential, combination overtones, hot bands in polyatomic molecules. 3
  - 4.4 **Vibrational rotation spectroscopy:** Fine structure in diatomic molecules, break down of Born-Oppenheimer approximation, effects due to spin, parallel and perpendicular vibrations 3
  - 4.5 **Raman spectra:** Polarizability ellipsoid, rotational and vibrational Raman spectra. 2
  - 4.6 **Electronic spectroscopy:** Born Oppenheimer approximation, molecular progression and term symbols, Frank-Condon principle, dissociation energies, oscillator strengths, rotational fine structure.. 3
  - 4.7 **ESR and NMR spectroscopy:** Principles, spin densities and factors affecting g values 3

## CHT 2103. Separation Chemistry

1. Absorption, adsorption and ion exchange processes. 2
2. **Distillation:** Vapour-liquid equilibria. Normal and fractional distillation, batch and continuous distillation. Azeotropes and separation of azeotropes. Steam distillation. 5
3. **Precipitation:** Normal, fractional. Sedimentation and crystallization 2
4. **Sublimation** 1
5. **Solvent extraction:** Liquid-liquid, leaching. Dissociative and reactive separations. 3
6. Filtration and centrifugation. 2
7. Membrane processes: MF, UF, Osmosis and RO, pervaporation. 3
8. **Chromatography:** Types
  - GC:** Columns and column performance, detectors, derivatization, 4
  - HPLC:** Principles, columns including chiral columns, detectors. 3
  - Ion exchange chromatography, exclusion chromatography, gel permeation chromatography, HP-TLC 4
- 9 Electrophoresis 1

## Practicals:

### CHP 2503 Physical Chemistry Laboratory- III

Construction of Z matrix, electronic structure and bonding analysis using GAMESS, molecular modeling, interpretation of spectral data, interpretation of XRD data, study of complex phase diagrams- micro emulsion systems Maxwell speed distribution by numerical integration, study of rotational probability distribution, computer applications in data analysis.

### CHP 2403 Organic Chemistry Laboratory-III

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

### CHP 2101 Analytical Chemistry Laboratory

Use of instrumental methods: GC, UV-VIS, IR, HPLC, MS, Corrosion studies, Cyclic voltametry,

## SEMESTER IV

### CHT 2404. Bioorganic chemistry

- 1. Proteins:** Amino acid sequence, method of determining the sequence, Peptide synthesis, Biologically active peptides, protein conformation. **4**
- 2. Nucleic acids:** Conformation and function of DNA and RNA, genetic code, mutation, recombinant DNA, DNA synthesis, DNA biosynthesis and related drugs. **6**
- 3. Enzymes:** Nomenclature and classification, purification, Concept of active site, affinity labeling and enzyme modification by site-directed mutagenesis, Microbial reactions, enzymes in organic solvent, enzyme mechanisms, chymotrypsin, ribonuclease, lysozyme and carboxypeptidase A, cytochrome 450, cofactors as derived from vitamins, coenzymes, prosthetic groups, apoenzymes.  
Structure and biological functions of - coenzyme A, thiamine pyrophosphate, pyridoxyl phosphate, NAD<sup>+</sup>, NADP<sup>+</sup>, FAD, FMN, flavin dinucleotide, vit B12. **9**
- 4. 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 **5**
- 5. Biogenesis and biosynthesis of natural products:**  
Primary and secondary metabolites, methods used in study of biosynthesis. Polyketide and Shikimic acid pathway, polyketides, terpenes and steroids, **4**
- 6. Lipids, structure, classification, characterization, metabolism. **2****

## CHT 2701. Chemical Process Economics

1. Demand and Supply.	3
2. Concepts of – taxes, interest, depreciation, inflation, working capital, operating cost, budget and balance sheet, profit	10
3. Cost analysis, price determination, project costs, cost of production.	8
4. Profit and loss account, annual report.	3
5. Project financing.	3
6. Marketing.	3

## CHP 2001 Seminar

Seminar topics will be given at the beginning of the second year (Semester III) by the Head of Department and the students will submit the compiled work at the end of the third semester and give a seminar at the beginning of the fourth semester. The submitted work and the seminar will be evaluated by a committee constituted for the purpose.

## CHP 2002 Project

### D. Special Papers

## CHT 2511. Catalysis

<b>1. Types of catalysis:</b> Heterogeneous and Homogeneous catalysis. Catalytic cycles	1
<b>2. Heterogeneous catalysis:</b>	17
2.1 Introduction: preparation methods, conversion and selectivity, catalyst deactivation and regeneration	
2.2 <b>Catalysis by surfaces:</b> Characterization and quantification of surface active sites, adsorption isotherms, kinetics of heterogeneous catalytic reactions reactions.,structure of adsorbed species, supported catalysts and metal support interaction ,	
2.3 <b>Catalysis in molecular scale:</b> Zeolites, mesoporous materials and clays as catalysts, shape selectivity	
2.4 <b>Characterization of catalysts:</b> Surface area, surface acidity and basicity, XPS, UPS, AES, EXAFS, XANES, XRD TPD etc.	
<b>3. Homogeneous catalysis:</b>	12
Advantages and disadvantages, homogeneous acid base catalysis. Hydrogenation, hydroformylation, hydrocyanation, hydrosilylation, Wilkinson catalysts, Chiral ligands and chiral induction, Ziegler-Natta catalysts	
<b>4. Organometallics as catalysts:</b> Bonding and structure transition metal complexes, applications in reactions such as hydrogenation, carbonylation, coupling reactions - Suzuki coupling, Heck coupling and related cross coupling reactions. Alkene oligomerization and metathesis. Catalytic oxidations and reductions, epoxidation, dihydroxylations, decarbonylation,	



olefin isomerization, arylation, polymerization, asymmetric synthesis, heterogenised homogeneous catalysts, phase transfer catalysis, catalysis in green chemistry

## CHT 2512. Industrial Engineering Chemistry

1. Types of Chemicals. Status of global and Indian Chemical Industry. **1**
2. Operation and Processes in Petrochemical Industry **3**
3. **Coal:** Types. Carbonization, liquefaction, gasification. **2**
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. **24**

## CHT 2411. Natural Products

1. **Steroids:** Cholesterol, bile acids, steroidal hormones, Synthesis of 16-DPA from cholesterol, synthesis of commercially important steroids from 16-DPA, synthesis of Taxol. **10**
2. **Carbohydrates:** anhydro-, amino-, branched chain, unsaturated sugars. Oligo and poly-saccharides. Degradation and reactions of sugars. Sugars as raw materials. Configurational assignments of monosaccharides, Amylose and amylopectin, cellulose, hemicelluloses, glycogen, inulin, sulphated polysaccharides **10**
3. **Plant pigments:** carotenoids, anthocyanins, flavones **3**
4. **Prostaglandins:** Structure determination and synthesis of PGE1 and PGF1. Insect pheromones and insect growth regulators **3**  
Plant growth regulators. **3**
5. **Antibiotics:** cephalosporin, en-dyne-antibiotic. **4**

## CHT 2412. Polymer Chemistry

1. **Monomers:** Their sources and synthesis **3**
2. **Methods of polymerization:** Bulk, Solution, Suspension, Emulsion, Addition, Melt, Condensation. **2**
3. **Mechanisms of polymerization:** Ionic and coordination polymerization. Step-Grown vs chain growth. Degree of polymerization. **3**
4. **Properties of polymers:** Viscosity, end-group analysis, hardness, abrasion resistance Structure and properties: Morphology and crystallinity, Molecular weight distribution- Number and weight average molecular weight. Polydispersity, crystallinity. Glassy state - Glass transition temperature  $T_m$  and  $T_g$ . Stereochemistry. **8**
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 **2**

### **CHT 2413. Heterocyclic chemistry**

**1. Nomenclature:** Nomenclature of heterocyclic compounds including polycyclic compounds. Strain, polarity, tautomerism, aromaticity in heterocyclic compounds, **4**

**2. Small rings:** aziridines, thiirane, azetidine, oxetane, thietanes **4**

**3. Five membered:** Diazoles, oxazoles and thiazoles. **5**

**4. Six membered:** Diazines, triazenes, pyranes and pyrones **5**

**5. Seven membered:** Diazepines **4**

**6. Fused ring:** Benzofurans, benzopyrans, benzodiazepines, indole, quinolines and isoquinolines, purines **5**

(Synthetic strategies based on retrosynthesis and reactions of the above heterocycles)

**7. Applications of heterocyclic compounds as drugs, dyes, optical brighteners, perfumes, etc** **3**

### **CHT 2414. Radicals, Photochemistry, and Pericyclic Reactions**

**1. Radicals** **8**

**1.1 Radicals:** Generation of radicals. Nucleophilic and electrophilic radicals. Characteristic reactions - Free radical substitution, addition to multiple bonds.

**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: S<sub>N</sub>Ar reactions

**2. Photochemistry** **10**

**2.1 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

**2.2 Photosensitized reactions, chemiluminescence.** Photosensitization, quenching, quantum efficiency and quantum yield.

**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, adamantane, etc. Flash photolysis and lasers

### **3. Pericyclic reactions** **12**

**3.1 Types:** Thermal and photochemical. Cycloaddition, electrocyclic reactions, sigmatropic rearrangement, 1,3-dipolar reactions, [3,3] shifts

**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.

**3.4 Electrocyclic reactions:** ring opening of cyclobutenes, ring closure of hexatrienes, cyclopropyl halide solvolysis; charged systems.

**3.5 Sigmatropic rearrangements:** [1,n] H-atom shifts, Cope and Claisen rearrangements, ene reaction.

3.6 Application of pericyclic reaction in synthesis.

## **CHT 2513. Surface and Interfacial Chemistry**

1. Concept of surface free energy and surface tension, interfacial tension and interfacial free energy, surface excess. **2**

**2. Liquid surfaces:** **8**

**2.1 Thermodynamics of liquid surfaces:** Gibbs adsorption isotherm, spreading coefficient and wetting phenomena.

**2.2 Thermodynamics of curved surfaces:** Young, Laplace, Kelvin, and Thomson equations.

2.3 Bubbles and foams, homogeneous and heterogeneous nucleation.

3. Potentials of interfaces, interfacial viscosity. Insoluble monolayers, LB films and molecular self assembly. **3**

**4. Group Theory :** Symmetry and symmetry operations, symmetry elements, character tables. **4**

**5. Crystal structure:** Symmetry elements, symmetry point groups and space groups, unit cells, Miller indices, Bravais lattices. Crystal structure determination by x-ray, electron and neutron diffraction.

**6. Solid surfaces:** **8**

6.1 Surface energy and imperfections, adsorption at solid surfaces

6.2 **Solid- liquid interfaces:** Work of adhesion and cohesion, wetting and contact angles, adsorption from solution at solid/ liquid interfaces, critical surface tension.

6.3 **Electrical properties of double layers:** Models of EDL, colloidal stability, DLVO theory, electrokinetic phenomena, zeta potential- measurement and applications.

## CHT 2415. Developments in Organic Synthesis

<b>1. Activation of small molecules:</b> CO, CO <sub>2</sub> , O <sub>2</sub> , CH <sub>4</sub> , NH <sub>3</sub> . C-C bond activation	<b>6</b>
<b>2. New energy sources:</b> Cavitation and sonochemistry, use of microwaves Microorganisms and enzymes in Organic synthesis High pressure reactions	<b>5</b>
<b>3. New solvents:</b> Water, ionic liquids, supercritical fluids Chemicals derived from methane, carbon monoxide, synthesis gas and biomass.	<b>6</b>
<b>4. Supported reagents and catalysts:</b> Merrifield resin and its applications. Clay supported reagents.	<b>6</b>
<b>5. Electrochemical synthesis:</b> Cathodic reductions and anodic oxidations	<b>3</b>
<b>6. Multicomponent reactions.</b>	<b>3</b>
7. Microreactor technology	<b>1</b>

## CHT 2611. Green Chemistry

1. Safety with respect to – toxic chemicals, pressure, temperature, dust, vapors and mist, transport, handling, storage. .	<b>5</b>
2. Hazard identification, assessment and safety audit. HAZOP and HAZAN. Air and water quality standards	<b>2</b>
3. Air pollution: Generation and effects of CO, CO <sub>2</sub> , NH <sub>3</sub> , SO <sub>2</sub> , NO <sub>x</sub> , Hydrocarbon, particulates.	<b>4</b>
4. Water pollution: Chemical, physical and biological characteristics of water pollution: DO, BOD, COD, and Chlorine. Water treatments – Oxidations, chlorination, ozonation.	<b>5</b>
5. Treatment of industrial waste.	<b>3</b>
6. Remedial measures to curb pollution	<b>3</b>
7. Green chemistry	<b>5</b>
8. Case studies	<b>3</b>

## CHT 2514. Quantum Chemistry

1. Mathematical review, matrices and determinants, polar, Cartesian and spherical coordinates, Legendre and Laguerre polynomials, linear and Hermitian operators	<b>5</b>
2. Basic postulates of quantum mechanics- state functions, operators, Eigen value equations, coverage value, time dependent Schrodinger equation, orthogonal and orthonormal functions Free particle and particle in a box, degeneracy, rigid rotor and harmonic oscillator, hydrogen atom, angular momentum, electron spin, spin orbit coupling	<b>7</b>
3. Approximation methods – variation theorem- application to helium atom, antisymmetry, Slater determinant wave functions.	<b>4</b>
4. Born-Oppenheimer approximation, Hartree Fock method (RHF and UHF), Kooper theorem, Roothan's equation.	<b>4</b>

5. Models of chemical bonding- MO and VB theories, applications to diatomic molecules such as H<sub>2</sub> and H<sub>2</sub><sup>+</sup>, basis sets **3**
6. Huckel theory and its applications , Walsh diagrams and molecular geometry, introduction to DFT **4**
7. Molecular mechanics- force field development, QM and MM methods **3**

### **CHT 2416. Unit Processes in Organic Synthesis**

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. **16**
3. Principles of polymer chemistry and polymerization practice. **2**

### **CHT 2417. Pharmaceutical Chemistry**

1. **Introduction to Drugs:** Nomenclature, Pharmacophore, Prodrug, Half – life efficiency, LD<sub>50</sub>, ED<sub>50</sub>, Therapeutic Index. Receptors, Drug – receptor interaction, Drug Potency, Bioavailability, Drug toxicity, Drug addiction. **6**
2. Absorption, disposition, elimination of drug. Metabolism of drugs. **3**
3. Routes of Drug administration and dosage forms **2**
4. Study of following classes of drugs with respect to – nature of disease, important drugs with synthesis, their mode of action: CNS Drugs, Analgesics and Antipyretics, Anti-inflammatory Drugs, Antihistaminics, Cardiovascular Drugs, Antidiabetic agents, Antiparkinsonism Drugs, Drugs for respiratory system, Antibiotics, Antimalarials, Antiamoebic Drugs, Anthelmintics, Antitubercular, Antileprotic drugs, Anti Neoplastic Drugs, Anti HIV Drugs. **19**

### **CHT 2418. Pesticides**

1. Insect biotypes, damage to plant by insects, host-plant resistance, **3**
2. Pests and diseases of - crop plants, pulses & vegetables, forage crops, Oil seed crops, cash-crops. Fungal Diseases of the crop plants **4**
2. Tactics and strategies of pest management (IPM). **2**
3. Synthesis of some important pesticides **9**
4. Insect attractants, chemosterilents and repellents, allelochemicals and pheromones. **4**
5. Plant protection appliances: Duster, Controlled release pesticides **2**
6. Pesticide residues and toxicology, Advances in pest control **2**
3. Recent advance in pest control: Green Chemistry in pesticides Light activated pesticides, pro-pesticides, genetic control, and chemosterilants **4**

## CHT 2515. Electrochemistry

1. Electrochemistry of solutions- strong and weak electrolytes, 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, Bjerrum theory **9**
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. **7**
3. **Corrosion** – chemical and electrochemical corrosion, Pourbaix diagram, differential aeration corrosion, prevention of corrosion- corrosion inhibitors, sacrificial electrodes. **5**
5. Kinetics of electrode reactions, electrical double layer, electro capillarity, electrokinetic phenomena, zeta potential and its applications. Electrochemical synthesis. **4**
6. **Industrial electrochemistry:** Electrodeposition, electroplating, throwing power, deposition of metals electro synthesis, fuel cells and batteries, poly electrolytes. **5**

## CHT 2419. Chemistry of Oleochemicals

1. Sources of oils and fats: Vegetable, animal, marine and algae sources. Methods of isolation/extraction, oils and fats as feedstock for oleochemicals. **3**
2. Chemistry, including methods of synthesis, of – Fatty acids, fatty alcohols, fatty esters, fatty amines, dimer acids, glycerol, telomer acids, synthetic dibasic acids. **12**
3. Study of following processes at molecular level and study of the physico-chemical principles involved: Esterification, catalytic hydrogenation, esterification and transesterification, hydroformylations, amination, fat splitting, metathesis **12**
4. Glycerol based chemicals. **2**
5. Biodiesel. **1**

## CHT 2516. Chemistry of Surfactants

1. Introduction: General structure, types, nomenclature **2**
2. Emulsions, microemulsions, gels, foams, LB films. **3**
3. Properties of surfactant solutions. Experimental methods involved. **5**
3. Aggregational behavior: Formation of micelles, vesicles, living polymers. Effect of additives on the aggregational behavior. **4**
4. Synthesis of surfactants: Synthesis of hydrophobes, functionalisation of hydrophobes. **8**
5. Structure-property relationship in surfactants **3**
6. Hydrotropes: Nature, structure, behavior, applications. **2**
6. Applications of surfactants **3**

## CHT 2517. Computational Chemistry

- 1. Fortran/C Programming and Numerical Methods:** Advanced programming features of FORTRAN/C. Basic theory, discussion of algorithms and errors for the following numerical methods. Examples from chemistry should be selected for illustrating the methods. The teacher may select ANY THREE of the following subtopics considering the background of students, available time etc. **6**
- 2. Solution of Equations:** Bisection, regular falsi, Newton-Raphson and related methods for solving polynomial and transcendental equations. Convergence. Errors and ill-conditioning. **4**
- 3. Linear Simultaneous Equations:** Gaussian elimination, Gauss-Seidel method, Gauss-Jordan method. Pivoting strategy, Errors and ill conditioning. **4**
- 4. Eigenvalues and Matrix Diagonalization:** Jacobi and Householder methods, analysis or errors. **3**
- 5. Interpolation:** Newton forward and backward difference, central differenced formulae. Lagrange and Hermite interpolation. Polynomial wiggle problem. **5**
- 6. Numerical Integration:** Solution of simple differential equations by Taylor series and Runge-Kutta methods. **3**
- 7. Numerical Integration:** Newton-Cotes formulae, Romberg integration, errors in integration formulae. The students should develop computer programs for some of the above numerical methods. **4**
- 8. Running of Advanced Scientific Packages:** Hands on experience of running a few selected advanced level scientific software packages. **1**

## CHT 2311. Nuclear Chemistry

1. Structure of atomic nucleus **2**
- 2. Radioactivity:** Determination of half life, radioactive decay kinetics, parent-daughter decay-growth relationships, Secular and transient equilibria, Compound nucleus theory, nuclear reactions, radioactivity, induced by heavy ions **5**
- 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. **8**
- 3. Radiation Chemistry:** Interaction of matter with radiation, radiation dosimetry-units and measurement of chemical dosimeters (Fricke and ceric sulphate dosimeters). 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. **8**
- 3. 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. **5**
4. Health and Safety Aspects **2**

## CHT 2420. Chemistry of Colorants

1. Spectral properties of colourants; Jablonski diagram; classification of dyes according to application and constitution; empirical treatment of colour and chemical constitution. **3**
2. Azo dyes – Diazotisation and coupling reactions; azoic colours; acid dyes; mono azo dyes; nitrodiphenylamine and anthraquinone classes; acid mordant dyes; azo metal complex dyes; direct dyes. **5**
3. Basic dyes – Diphenylmethane and triphenylmethane dyes and their heterocyclic analogues; triphenodioxazine dyes. **3**
4. Disperse dyes – Azo, anthraquinone, dinitrophenylamine, methane dyes; properties of disperse dyes in relation to constitution. **3**
5. Vat dyes – Indigoid, anthraquinonoid and polycyclic quinoid vat dyes; solubilised vat dyes. **4**
6. Sulphur dyes and sulphurised vat dyes. **3**
7. Introduction to classes of pigments; copper phthalocyanine and other colourants based on phthalocyanine. **3**
8. Reactive dyes – Chlorotriazine and other halo heterocyclic compounds; **3**
9. vinyl sulphone based dyes; high fixation, highly substantive, neutral fixing bifunctional reactive dyes; **2**
10. Mineral colours and oxidation colours **1**

## Reference Books

### CHT 2301. Chemistry of Main Group Elements & CHE 2301 Nuclear Chemistry

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 2401. 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 distributors
4. Advanced Organic Chemistry: Part A and B: Francis Carey
5. Advanced Organic Chemistry- Reaction and Mechanisms: Maya Shankar Singh: Pearson Education
6. Advance Organic chemistry, Reinhard Bruckner, Elsevier



### **CHT 2501 Thermodynamics 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. Thermodynamics of irreversible processes- Iila Progofine
5. Non equilibrium Thermodynamics- C.Kalidas and M.V.Sankaranarayana
6. Physical Chemistry, Maron and Pruton
7. Physical Chemistry, P.W. Atkins

### **CHT 2201. Material and Energy Balance**

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

### **CHT 2302. Materials Chemistry**

1. Introduction to Solids, Leonid V. Azaroff, Tata McGraw-Hill Publishing Company Ltd
2. Introduction to the Physics and Chemistry of Materials, Robert J. Naumann: Boca Raton: CRC Press
3. Material Chemistry: Bradley D. Fahlman: Springer-Verlag, New York
4. Materials Chemistry, Fahlman B.D., Springer

### **CHT 2303. Chemistry of Transition Metals**

1. Concise Inorganic Chemistry by J.D.Lee

### **CHT 2402. Stereochemistry**

1. Stereochemistry of organic compounds: Ernest L. Eliel, Samuel H. Wilen : A Wiley-interscience Publication

### **CHT 2502 Chemical Reaction Kinetics**

1. Modern Electrochemistry- J.O.M.Bockris and A.K.N.Reddy- Volumes I and II
2. Electrolytic solutions- R.A. Robinson and R.H. Strokes
3. Elements of Statistical Thermodynamics- L.K.Nash, Addison Wesley
4. Statistical Thermodynamics – B.J.McCelland, Chapman Hall
5. Thermodynamics and Statistical Thermodynamics – F.W.Sears, G.L.Salinger, Narosa
6. Physical Organic Chemistry: Neil S. Isaacs : ELBS

### **CHT 2101. Instrumental Methods of Analysis & CHT 302. Advanced Spectroscopy**

1. Spectroscopy, Pavia, L., Kriz, V., Cengage Learning India pvt
2. Instrumental methods of analysis: Hobart H. Willard, Lynne L. Merritt, John A. Dean, Frank A. Settle : CBS Publishers and Distributers
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 2202. Fundamentals of Fluid Flow and Heat Transfer**

1. Unit Operations in Chemical Engineering, McCabe and Smith
2. Heat Transfer, Kern D. Q.

### **CHT 2403. 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 2304. Organometallic Chemistry**

1. Organometallic Chemistry of Transition elements: F. P. Pruchnik: Springer
2. Organometallic Chemistry : R. C. Mehrotra: New Age International
3. Organometallic Chemistry: G. S. Sodhi: Ane Books Pvt. Ltd.
4. Organometallic reagents in Organic Synthesis: Paul R. Jenkins: Oxford Science Publications
5. Organometallics 1: Complexes with transition Metal-Carbon Sigma-Bonds: Manfred Bochmann: Oxford Science Publications
6. Organometallics 2: Complexes with transition Metal-Carbon pi-Bonds: Manfred Bochmann: Oxford Science Publications

### **CHT 2503. Molecular Spectroscopy and Bonding**

1. Fundamentals of molecular spectroscopy- C.N.Banwell
2. Introduction to Molecular spectroscopy- G.M.Barrow
3. Valence- C.A. Coulson
4. Introduction to quantum mechanics- L.Pauling and E.B.Wilson
5. Molecular spectroscopy- J.Machale

### **CHT 2103. Separation Chemistry - Unit Operations**

1. Unit Operations in Chemical Engineering, McCabe and Smith

### **CHT 2404. Bio-organic Chemistry**

1. Biotransformations in Organic Chemistry: Kurt Faber: Springer
2. Bioorganic Chemistry, Dugas, H, Springer
3. Bioorganic Chemistry, Soni, R.K. and Sharma, P, Saujanya Book, 2008

### **CHT 2701. Chemical Process Economics**

1. Chemical Process Economics - V.V. Mahajani and S.M. Mokashi, McMillan India

## **A. Elective Papers**

### **CHT 2511. Catalysis**

1. Principles and practice of heterogeneous catalysis - J.M.Thomas and W.J.Thomas-VCH publications, NY
2. Catalysis- concepts and green applications- Gadi Rothenberg-Wiley VCH
3. Homogeneous catalysis- mechanism and industrial applications- S.Bhadrri and D.Mukesh, John Wiley and sons
4. Design of heterogeneous catalysts –U.S.Ozkan (ed) – Wiley VCH
5. Introduction to surface chemistry and catalysis- G.A. Somarjai, Wiley and sons

### **CHT 2512 Industrial Engineering Chemistry**

1. Chemical Reaction Engineering, O. Levenspiel
2. Industrial chemistry by James Kent & Reigel.
3. Survey of industrial chemistry 2 Ed. by P.J.Chenier
4. Industrial chemicals: F.A.Lowheim and M.A.Moran.

### **CHT 2411 Natural Products**

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 2412 Polymer Chemistry**

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 2413 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 2414 Radicals, Photochemistry, and Pericyclic Reactions**

1. Frontier Orbitals and organic Chemical reaction: Ian Fleming
2. Advanced Organic Chemistry: Part A and B: Francis Carey

### **CHT 2513 Surface and Interfacial Chemistry**

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. Surface and Interfacial Chemistry by M.J. Rosen, Wiley Interscience.

### **CHT 2415. Developments in Organic Synthesis**

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

### **CHT 2611. Green Chemistry**

1. Theory and Practice: Anastas, P. T. and Warner J. C: New York Oxford University Press.
2. Green Chemistry: Design Chemistry for the Environment: Anastas, P. T, Williamson T. C.: Washington, D. C. American Chemical Society.
3. Green Chemistry: Frontier in Design Chemical synthesis and Process: Anastas, P. T., C. Williamson New York

### **CHT 2514. Quantum Chemistry**

1. Valence- C.A. Coulson, ELBS.
2. Introduction to quantum mechanics- L.Pauling and E.B.Wilson Quantum Chemistry, Ira N. Lavine
3. Quantum Chemistry, J.P.Low, K.A. Peterson, 3<sup>rd</sup> Edn., Elsevier
4. Essentials of computational chemistry, 2<sup>nd</sup> Edn., C.J.Cramer, Wiley
5. The basis of theoretical and computational chemistry, B.M.Rode, T.S. Hofer, Wiley VCH

### **CHT 2416. Unit Processes in Organic Synthesis**

1. Unit Operations: W.L.Badger.
2. Unit processes in organic synthesis: P.H.Groggins.

### **CHT 2417. Pharmaceutical Chemistry**

1. Medicinal and Pharmaceutical Chemistry; H. Singh and V.K. Kapoor.
2. Medicinal Chemistry by Malcolon Campbell and Ians B Lagbrough.
3. Foye's principles of Medicinal Chemistry by David A. Williams and Thomas L. Lemke.
4. Medicinal Chemistry; Principles and Practice by F.D. King.
5. Medicinal Chemistry by Burger A.; Wiley Interscience, New York.

### **CHE 2408. Pesticides**

1. Biological insect pest suppression by H.C.Cooper (Springer Verlag)
2. Pesticide chemistry by J.Miyamoto and P.C.Kearney (Pergamon)
3. Hand book of pest management in agriculture Vol.II by D. Pimentel.
4. Biological pest control by N.W. Hussey and N. Scopes (Glandford press)
5. Safer pesticides by E. Hodgson and R.J.Kuber (Dekker)
6. Insect sex pheromones by M.Jacobson (AP).
7. Pesticide production process- New Jersey.

### **CHT 2515. Electro-chemistry**

1. Electrochemistry in Non-aqueous solutions by K. Izutsu.
2. Electrochemistry by Wolf Vielstich, Carl H. Haman, Andrew Hamnett, Teresa Iwasita, 2007

### **CHT 2419. Chemistry of Oleochemicals**

1. Oleochemical Manufacture and applications - F.D. Gunstone & R.J. Hamilton(eds.)- Sheffield Academic Press-2001
2. Bailey's Industrial Oil and Fat production by Y.H. Hui

### **CHT 2516. Chemistry of Surfactants**

1. Surfactant Systems: their chemistry, pharmacy and Biology by D. Attwood and A.T. Florence-London, Chapman and Hall 1983.
2. Surfactant and Interfacial phenomena by M.J. Rosen, 2<sup>nd</sup> Edition, Wiley Interscience publications 1989
3. Surfactants: Chemistry and properties by Anhtony J O'LenickIllinois: Allured publication 1999

### **CHT 2517. Computational Chemistry**

1. Computational Chemistry, A.C. Norris, John Wiley.
2. Computer Programming in FORTRAN 77, R. Rajaraman, Prentice Hall.
3. Numerical Analysis, C.E. Frogberg, Macmillan.
4. Numerical Analysis-A Practical Approach, M.J.Maron, John Wiley.
5. Numerical Methods for Scientists Engineers, H.M. Antia, Tata McGraw Hill.

### **CHT 2311. Nuclear Chemistry**

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.Arnika (Wiley Eastern) 1987.
5. An Introduction to Radiation Chemistry-Spinks and Woods (Wiley, New York) 1990

### **CHT 2420 Chemistry of Colorants**

1. Colour Chemistry by H. Zollinger
2. Industrial Dyes by K. Hunger
3. Chemistry of Synthetic Dyes and Pigments by H. A. Lubs
4. Colour and Chemical Constitution by J. Griffiths