# Integrated M.Sc. – Ph.D. programme of the Dept. of Chemistry

## First Semester

<table>
<thead>
<tr>
<th>Code</th>
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<tr>
<td>CH 423</td>
<td>Organic Chemistry III</td>
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<td>Chemical Bonding and molecular Geometry</td>
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<td>Chemistry of Main Group Elements</td>
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Contact hours: 23  
Credits: 36

## Second Semester

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Contact hours: 30  
Credits: 42

## Summer at the end of 2\textsuperscript{nd} semester

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Credits: 12
### Third Semester

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Contact hours: 09  
Credits: 36

### Fourth Semester

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Contact hours: 12  
Credits: 34
Summer at the end of fourth semester

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Credits: 10

Fifth Semester

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Contact hours: 12
Credits: 24
Departmental electives I to III

Physical Chemistry

CH 504 Computational Chemistry
CH 550 Electrochemistry
CH 552 Interfacial Phenomena
CH 559 Solid State Chemistry and its Applications
CH 560 Quantum Chemistry
CH 576 Statistical Mechanics
CH 584 Biophysical Chemistry
CH 586 Structure and Properties of Materials
CH 5XY Macromolecular Crystallography

Organic Chemistry

CH-504 Computational Chemistry
CH 510 Heterocyclic chemistry
CH-528 Natural Products
CH-540 Drugs and Biologically active compounds
CH 546 Introduction to Biomolecules
CH-556 Polymer Sciences

Inorganic Chemistry

CH-522 Chemistry of Coordination Compounds
CH-524 Bioinorganic Chemistry
CH-574 Topics in Inorganic Chemistry-I
CH-578 Topics in Inorganic Chemistry-II
CH-582 Inorganic Photochemistry

Text/References


**CH 416   Physical Organic Chemistry  2106**


**Text/References**


**CH 418   Organic Chemistry Lab III  0044**

Chemical separation of ternary organic mixtures and characterization of the components. Simple one or two step preparations involving different techniques. Isolation of natural products.
Separation by Soxhlet and liquid-liquid extraction. Cation and anion exchange chromatography, column, thin layer and paper chromatography, gas-liquid and gel permeation chromatography. Fractional distillation.

**Texts/References**


A reappraisal of structure, stereochemical principles, properties and reactivity in organic compounds. Study of the following classes of reactions, nucleophilic substitutions, eliminations, electrophilic additions, electrophilic and nucleophilic substitution in aromatic compounds, nucleophilic addition, halogenation, and alkylation of carbonyl compounds. Reactions involving enamines, ester enolates and active methylenes.


**Texts/References**


Postulates of quantum mechanics; hermitian operators; complete set. Derivation of the uncertainty relations. Exactly solvable problems, orbital angular momentum, and the hydrogen atom. Spin, spin orbitals, and characteristics of a many-electron wave function.

Variation theorem, variation method, the linear variation method, and the non-crossing rule. Applications: Many-electron atoms, self-consistent field, atomic orbitals, Slater Type Orbitals, Slater exponents and the periodic properties of elements; LCAO-MO, Hückel orbitals; Born-Oppenheimer approximation, Potential energy surface, Hellman-Feynman theorem; Hydrogen molecule ion, Hydrogen molecule; Qualitative molecular orbitals for homo- and hetero-nuclear diatomics, isoelectronic principle, hybrid orbitals, and Walsh molecular orbital diagram.

Time-independent perturbation theory - Rayleigh-Schrödinger formulation. Applications: Zeeman effect, Stark effect, crystal field splitting, and simple ligand field treatments.

The valence bond treatment of hydrogen molecule; Resonance; Polarity and dipole moment; Electronegativity; Valence-bond wave functions for polyatomic molecules.

**Texts/References**


**Texts/References**


**CH 427 Chemical and Statistical Thermodynamics**

Applications of thermodynamic functions; partial molar quantities; non ideality and activities; chemical equilibria. Ensembles, MB, BE and FD distributions; Partition functions and their relationships to thermodynamic functions and equilibrium constant; Virial coefficients; Lattice Models; Introduction to non-equilibrium thermodynamics; Onsager’s reciprocity relations.

**Text / References**


**CH 429 Modern Methods of Analysis**

Evaluation of reliability of analytical data and statistics in chemical analysis. Expression of results to significant figures. Sampling and preparation of sample for analysis. Introduction to optical methods, ultraviolet, visible, infrared spectrophotometry and fluorimetry. Atomic absorption and flame emission spectroscopy. Scattering of radiation, nephelometry, turbidimetry and Raman Spectroscopy. Electroanalytical methods such as voltammetry, polarography, amperometry, conductometry and high frequency titrations. Thermogravimetry
and differential thermal analysis. Introduction to interphase separations with special reference to chromatography. Gas chromatography and HPLC.

**Text References**


**CH 432  Inorganic Chemistry Lab III  0 0 4 4**

Complexometric titrations by masking and demasking reactions. Estimations by nephelometry, fluorimetry, simultaneous spectrophotometry, atomic absorption spectroscopy. Determination of composition of complexes in solution. Synthesis and characterization of transition metal complexes (including organometallic compounds) and their study by spectral, magnetic and thermal methods.
CH 433 Physical Chemistry Lab II  0 0 4 4

Phase equilibria, viscosity and molecular weight of polymers, surface tension, reaction kinetics (rates, order of reaction, influence of ionic strength), use of thermocouples, transition temperature determinations, self generated experiment.

CH 434 Physical Chemistry Lab III  0 0 4 4

Determination of the following physical quantities: partial molal volumes, dipole moments, activities by freezing point, quantum yields, heats of vaporisation and depressions of freezing points of solutions, velocity constant and activation energy. Electrodes with different substrates for H₂ evolution, photoelectrochemical solar cells. Vacuum measurement. IR spectrum of HCl, Use of M.O. theory, solution of Schrodinger equation for polyatomics.

CH 437 Chemistry of Transition Elements  2 1 0 6

General chemistry of the transition elements, lanthanides and actinides including atomic nuclei and nuclear reactions, coordination chemistry including theories of metal-ligand bonding, spectral and magnetic properties, organometallic compounds of transition elements, role of transition metal ions in biological processes.

Texts/References


CH 438 Chemistry of Main Group Elements  2 1 0 6

Chemistry of non-transition elements, stereochemistry and bonding in non-transition elements and compounds. Solvents, solutions, acids and bases, brief review of inorganic chains, rings and
cages, organometallic compounds of non-transition elements, role of non-transition elements in biological processes.

Texts/References

CH 481: Chemistry and Computers

Numerical computing using a high level language like FORTRAN/C: Programming principles using loops, arrays and functions; use of libraries; Numerical methods: truncation and round off errors; roots; interpolation; differentiation and integration; linear equations, matrix operations; curve fitting; ODEs; optimization; Application of numerical methods to chemical problems.

Text/References
CH 502  Synthesis and characterization of Inorganic Compounds.  2106

Preparative chemistry of compounds of main group and transition elements including inorganic chains, rings, cages, clusters, halogen and rare gas compounds. Experimental problems encountered in the synthesis, isolation, purification, characterization and identification of inorganic compounds. Physical methods for characterization, PES, EXAFS, Mossbauer spectroscopy, magnetic susceptibility and cyclic voltammetry.

Text/References

CH 504 Computational Chemistry  1046

A brief outline of molecular mechanics, semi-empirical approximations, ab initio methods, basis sets and Z-matrix; Application of these computational methods for prediction of structural and electronic properties of molecules by using standard programs; FMOs in organic chemistry, crystal and ligand field calculations, computation of potential energy surfaces. Conformational analysis by molecular mechanics; Dynamical and structural studies of molecules using molecular dynamics simulations; Monte Carlo simulations of molecules.

Texts/References:
A review of various synthetic methods in organic chemistry: Formation of C-C, C≡C, C=C bonds and various rings (namely 3, 4, 5, 6, 7 and 8-membered ring) with special emphasis on utility of several types of organometallic reagents. Selected syntheses of natural and unnatural products having these ring systems. A concise introduction to various aspects of asymmetric synthesis followed by detailed discussion on resolution, chiral auxiliaries, chiral ligands, chiral catalysts, and organocatalysts with specific examples. A brief discussion on biosynthesis and biomimetic synthesis with selected examples from monoterpnes, sesquiterpenes, diterpenes, steroids, and alkaloids. Introduction of domino and tandem reaction concepts with a detailed discussion on selected examples.

Texts/References:

General comparison of organic reactions carried out in laboratory and organic reactions observed in biological systems. Nature of biomolecular interactions, physical concepts. Stereospecificity and rate enhancement in enzyme catalysed reactions. Discussion on non-availability of electrophilic sites in enzymes and their presence in co-enzymes. Following reactions will be discussed (comparing the usual mechanism to enzyme catalysed mechanism): hydrolysis of esters, amides, phosphoesters, etc. C-C and C=C bond formation, oxidation, reduction and decarboxylation. Remote functionalisation cyclisation reactions. Biomimetic reactions. Hydrophobicity, organized assemblies. Supramolecular structure, drug design.

Text/References
CH 510  Heterocyclic chemistry

Introduction to heterocyclics and their importance. Nomenclature of ring systems, structure, reactivity and synthesis of reduced three, four, five and six membered oxygen, nitrogen and sulphur heterocyclics; aromatic heterocyclics, 5-membered, 6-membered and polyhetero ring systems - indole, azoles and diazines. Constitution and configuration of simple sugars, chemical reactions of monosaccharides and their cyclic anomers.

Texts/References


CH 521 Interpretative Molecular Spectroscopy

Mass spectrometry, the production and analysis of positive ions, molecular ions, application of isotopic abundance measurements, fragmentation modes and rearrangement of ions. Mass spectra of certain chemical classes. Electronic spectroscopy (UV-visible, fluorescence and phosphorescence): Simple chromophoric groups, conjugated and aromatic systems. Characteristic absorption of organic and inorganic compounds. Infrared spectroscopy: Characteristic group frequencies of organic and inorganic molecules. Nuclear magnetic resonance spectroscopy of compounds containing $^1$H, $^{13}$C, $^{19}$F and $^{31}$P nuclei. Identification of organic and inorganic compounds using combination of spectral data.

Text/References


**CH 522  Chemistry of Coordination compounds**


**Text/References**


**CH-523  Molecular Spectroscopy**

Introduction to spectral energy domains and measurement of spectra, Implications of discrete energy levels, Population of States – Boltzman Distribution, Interaction of radiation with matter, origin of linewidths in molecular spectra, Transition dipole moment and Fermi’s Golden Rule, Einsteins Coefficients, Lasers and Masers;

Rotational (Microwave) spectroscopy, Molecular vibrations - Infrared spectroscopy, Normal mode analysis, Raman Scattering, Selection Rules from Group Theory, Molecular electronic spectra, Photophysical processes, Non-Linear Spectroscopy, Nuclear Magnetic Resonance, Relaxation times, FT-NMR, spin-spin coupling, ESR, Nuclear Quadrupolar Resonance.

**Text/References**


CH-524  Bioinorganic Chemistry  2106


Text/References

CH 528  Natural Products  2106

Terpenoids: Classification, structure, chemistry and biogenesis of some important mono; sesqui, di, and triterpenes.
Steroids: Sterols and bile acids, estrogens, androgens, gestogens and adrenocortical hormones. Hormone production. Cardiac glycosides. Steroidal triterpenes; biogenesis of steroids and correlation with terpenoids.

Alkaloids: Characteristic reactions, general methods of degradation, structure and chemistry of some well-known alkaloids.

Natural Pigments: Flavones, flavanones, isoflavones, xanthones, quinones, pterins, chlorophyll and haemin.

Carbohydrates: Stereochemistry, reaction and conformation of monosaccharides, deoxy and aminosugars, hexonic acid and vitamin C, disaccharides, polysaccharides, inositol; gangliosides and other glycosides. Chemistry of vitamins A, B, C and E.

Text/References


CH 540 Drugs and Biologically Active Compounds

Drug receptor interactions. Approaches to drug design. Drug metabolism. A few drugs from each of the following groups will be discussed.

Analgesics, antidepressants, antipsychotics, antiinflammatory agents, cardiovascular agents, diuretics, antibacterials, antibiotics, antivirals, antimalarials, antiamoebics, drugs for neoplastic diseases.

Vitamins: A, B1, B2, B6 niacin, folic acid, dantothenic acid, biotin, B12, C, D, E and K. Hormones: Thyroid hormones and antithyroid drugs. Steroid hormones and some important steroidal drugs.
**Texts/References**


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**CH 546  Introduction to Biomolecules**


**Texts/References**


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**CH-547  Organometallic Chemistry**

Historical background, factors controlling metal-carbon bond formation, methods of M-C bond formation, comparative survey of structure and bonding of metal alkyls and aryls, complexes with p acids, CO and related ligands, complexes with olefins, acetylenes and related unsaturated molecules, catalytic properties of mononuclear compounds, stereochemical non-rigidity in organometallic compounds, boranes, carboranes and metalallocarboranes, bimetallic and cluster complexes, structure and applications in catalysis, applications of organometallic
compounds in organic synthesis, enantioselective synthesis via organometallic compounds, importance of organometallic compounds in certain biological systems.

**Text/references**


**CH 550 Electrochemistry**


**Text/References**


CH 552  Interfacial Phenomena


Text/References

CH 556: Polymer Science

Introduction and applications of polymers, molecular weight distributions, various experimental methods (GPC/SEC, solution viscosity, VPO, light scattering) to determine relative and absolute molecular weight distributions, chain growth and step growth mechanisms and kinetics, ionic polymerization, living polymerization, stereochemistry of polymers, free radical copolymerization (random, block, alternate and graft copolymers), kinetics and mechanisms of free radical copolymerization, polymerization conditions and polymer reactions, thermal, mechanical and solution properties of polymers, thermoplastics, thermosets and elastomers, conducting polymers, branched polymers (star, dendritic and hyperbranched polymers).

Text/References
CH 557  Topics in Chemistry                                                                     3 0 0 6

Structure of solids, surfaces, interfaces and soft matter, electronic structures, structure and properties of nanocrystals. Introduction to polymers; physical properties of polymers; classification of polymers based on kinetics and methods to characterize polymers. Structural Inorganic Chemistry: Basic aspects of single crystal X-ray diffraction, methods of structure determination and interpretation of structures.

Homogeneous catalysis: Metal ions in organic transformation, basic principles, activation energy, essential steps in catalysis, catalytic transformation to useful organic compounds.

Text/References
P. J. Flory, Principles of Polymer Chemistry, Cornell University Press, 1953
M. Chanda, Advanced polymer chemistry: a problem solving guide, Marcel Dekker, 2000

CH 559 Solid State Chemistry and Its Applications                                            2 1 0 6


Electronic structure of solids: Fermi level, Bloch orbitals, energy bands, Brillouin zone. Electric and magnetic properties of solids: insulators, semiconductors, conductors and Fermi surfaces; superconductivity; polarization, refractive index, dielectrics and ferroelectrics; diamagnetism and paramagnetism; ferromagnetism, ferrimagnetism and antiferromagnetism. Molecular metals, phosphors and solid state lasers.

Texts/References


**CH 560  Quantum Chemistry**


**Texts/References**


**CH-574  Topics in Inorganic Chemistry-I**


**Text/References**


CH-576 Statistical Mechanics


Texts/References


CH-578 Topics in Inorganic Chemistry - II


Text/References

CH 582 Inorganic Photochemistry 2106


Text/References

CH-584 Biophysical Chemistry 2106


Text/References


**CH 586  Structure and Properties of Materials**


**Text/References**


**CH 588  Organic Synthesis**


**Text/References**


**CH 5XY Macromolecular Crystallography**

Basic Diffraction Theory, Bragg’s law, Miller Indices, Laue Equations, Protein and Nucleic acid Structure, X-ray major sources and production, Xray detectors, Crystallization techniques and principles, symmetry and space groups, reciprocal space, Fourier transform, structure factor equation, phase problem, data collection and processing, methods of structure determination, heavy atom solutions like direct methods, patterson methods, Multiple Anomalous diffraction, Single Anomalous diffraction, sulphur phasing, Isomorphous replacement, Molecular replacement, structure refinement and validation, structure deposition, elucidation of mechanism from structure, biological crystallography examples of virus, ribosomes, membrane proteins, macromolecular assemblies

**Suggested Text:**

*Principles of protein x-ray crystallography* Jan Drenth,

Crystallography Made Crystal Clear, Gale Rodes

*Structure determination by X-ray crystallography* M. Ladd and R Palmer

**CH-593 : M. Sc. Project**

**CH-594 : Project**