# M. Sc. Syllabus

## Semester - 1

<table>
<thead>
<tr>
<th>Course No</th>
<th>Course Name</th>
<th>L-T-P-C</th>
</tr>
</thead>
<tbody>
<tr>
<td>CH 410</td>
<td>Transition and Non-transition Metal Chemistry</td>
<td>3-1-0-8</td>
</tr>
<tr>
<td>CH 415</td>
<td>Inorganic Chemistry Laboratory</td>
<td>0-0-9-9</td>
</tr>
<tr>
<td>CH 420</td>
<td>Principles of Organic Chemistry</td>
<td>3-1-0-8</td>
</tr>
<tr>
<td>CH 430</td>
<td>Quantum Chemistry</td>
<td>3-1-0-8</td>
</tr>
<tr>
<td>CH 431</td>
<td>Group Theory and Spectroscopy</td>
<td>3-1-0-8</td>
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**Total Credits:** 12-4-9-41

## Semester - 2

<table>
<thead>
<tr>
<th>Course No</th>
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<tbody>
<tr>
<td>CH 411</td>
<td>Inorganic Reaction Mechanism and Organometallals</td>
<td>3-1-0-8</td>
</tr>
<tr>
<td>CH 421</td>
<td>Organic Reactions Mechanisms</td>
<td>3-1-0-8</td>
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<tr>
<td>CH 425</td>
<td>Organic Chemistry Laboratory</td>
<td>0-0-9-9</td>
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<tr>
<td>CH 432</td>
<td>Chemical Dynamics and Electrochemistry</td>
<td>3-1-0-8</td>
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<tr>
<td>CH 433</td>
<td>Applications of Spectroscopy</td>
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**Total Credits:** 12-4-9-41

## Semester - 3

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<th>Course No</th>
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<tbody>
<tr>
<td>CH 500</td>
<td>Graduate Seminar</td>
<td>0-0-2-2</td>
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<tr>
<td>CH 511</td>
<td>Principles of Bioinorganic Chemistry</td>
<td>3-1-0-8</td>
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<tr>
<td>CH 520</td>
<td>Concepts in Organic Synthesis</td>
<td>3-1-0-8</td>
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<tr>
<td>CH 521</td>
<td>Modern Techniques and Scope of Chemical Biology</td>
<td>3-1-0-8</td>
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<tr>
<td>CH 530</td>
<td>Classical and Statistical Thermodynamics</td>
<td>3-1-0-8</td>
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<tr>
<td>CH 535</td>
<td>Physical Chemistry Laboratory</td>
<td>1-0-8-10</td>
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**Total Credits:** 13-4-10-44

## Semester 4

<table>
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<th>Course No</th>
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<tbody>
<tr>
<td>CH 501</td>
<td>Computer in Chemistry</td>
<td>2-0-1-5</td>
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<tr>
<td>CH 600</td>
<td>Project</td>
<td>0-0-18-18</td>
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<tr>
<td>CH 6xx</td>
<td>Elective I</td>
<td>3-1-0-8</td>
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<tr>
<td>CH 6xx</td>
<td>Elective II</td>
<td>3-1-0-8</td>
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**Total Credits:** 8-2-19-39

List of Elective Courses

- CH 640 Principle and Applications of Luminosence Spectroscopy
- CH 615 Advanced Organometallic Chemistry
- CH 637 Advanced Quantum Chemistry
- CH 616 Bioinorganic Chemistry
- CH 625 Art in Organic Synthesis
- CH 626 Modern Reagents in Organic Synthesis
- CH 637 Advance Quantum Chemistry
- CH 628 Advances in Nucleic Acid and Lipid Chemistry
Syllabus

**CH-410 : Transition and Non-transition Metal Chemistry**

Non-transition Metal Chemistry: Synthesis, Properties, Structure and Bonding of:
Nitrogen, Phosphorous, Sulfur, Pseudohalogen, Interhalogen and Xenon Compounds; Boranes, Carboranes, Metallocarboranes, Borazines, Phosphazenes, Sulfur-Nitrogen compounds, silicates, silicones. Iso- and Hetero-poly anions.

**Text Books:**


**References:**


**CH-415: Inorganic Chemistry Laboratory**

Synthesis and characterization of inorganic compound including co-ordination complexes, assemblies.
Synthetic methods: solution chemistry, solid state synthesis, sol-gel methods, multi step synthesis, preparation of isomers, synthesis under inert atmosphere, electrosynthesis.
Characterization: quantitative and qualitative determination of ligand and metal, use of spectral techniques (UV - visible, IR, NMR, ESR, magnetic moment,
analytical methods (conductance, TG, DSC, cyclic voltametry, coulometry).

Text Books:

2. Synthetic methods of organometallic and inorganic chemistry ed. by Wolfgang A. Herrmann, Georg Thieme Verlag, New York, 1997, Vol 7 and 8

CH-420: Principles of Organic Chemistry 3 1 0 8

Structure and Bonding: Review of basic principles of structure and bonding, application of acid base concepts, HSAB theory, aromaticity and antiaromaticity, Hückel’s rule, anti-aromaticity, y-aromaticity, homo-aromaticity n-annulenes, heteroannulene, fullerenes, C-60, cryptates, Bonds weaker than covalent; addition compounds, inclusion compounds, crown ethers, cyclodextrins, catenanes and rotaxanes. Stereochemistry: Conformational analysis of cycloalkanes, effect of conformation on reactivity. Elements of symmetry, chirality, molecules with more than one chiral center, projection formulae (i) Fischer (ii) Sawhorse (iii) Newman (iv) Flying Wedge; threo and erythro isomers, methods of resolution, optical purity, enantiotopic and diastereotopic atoms, groups and faces, stereospecific and stereoselective synthesis. Asymmetric synthesis. Optical activity in the absence of chiral carbon. Reaction mechanism: Structure and Reactivity: Types of mechanisms, types of reactions, thermodynamic and kinetic requirements, Hammond postulate, Curtin-Hammett principle, transition states and intermediates, methods of determining mechanisms, isotopic effects. Generation, structure, stability and reactivity of carbocations, carbanions, free radicals, carbenes and nitrenes. Effect of structure on reactivity. The Hammett equation and linear free energy relationship (sigma-rho) relationship, Taft equation.


Text Books:
2. Stereochemistry of Carbon Compounds by E. J. Eliel, McGraw Hill

Reference:


**CH-430: Quantum Chemistry**

Review of essential mathematical concepts. Origin of the quantum theory. Postulates of quantum mechanics and Schrödinger equation; its application on some model systems viz., free-particle and particle in a box, tunneling, the harmonic oscillator, the rigid rotator, and the hydrogen atom. The variation theorem; linear variation principle; perturbation theory; applications of variational methods and perturbation theory to the helium atom. Ordinary angular momentum, generalized angular momentum, eigenfunctions, and eigenvalues of angular momentum operator, Ladder operator, addition of angular momenta. Spin, antisymmetry, Pauli exclusion principle, Slatter determinantal wave functions. Term symbol (RS and jj coupling) and spectroscopic states, term separation energies of pn and dn configurations, magnetic effects: spin-orbit coupling and Zeeman splitting. Virial theorem. Born-Oppenheimer approximation, VB and MO theory, H$_2^+$, H$_2$ molecule problem, Hückel molecular orbital theory and its application to ethylene, butadiene and benzene. Hybridisation and valence MOs of H$_2$O, NH$_3$ and CH$_4$. Introduction to the SCF.

Text Books:


References:

1. Quantum Chemistry by Ira N. Levine, Prentice Hall,

**CH-431: Group Theory and Spectroscopy**
Group Theory: Definition of group, symmetry, point groups, representation of
group, orthogonality theorem, irreducible representation, character table, direct
sum, direct product, derivation of projection operator. Spectroscopy:
Electromagnetic radiation and its interaction with matter. Uncertainty principle:
Natural line width and broadening.
Microwave; classification of molecules, rigid rotor model, selection rules, intensity
of spectral lines, effect of isotopic substitution. Stark effect. Infrared: Review of
harmonic oscillator, selection rules, vibrational energy of diatomic molecules, zero
point energy, force constant and bond strength; anharmonicity. Morse potential
energy diagram, vibration-rotation spectroscopy, P, Q, R, branches. Breakdown of
Born-Oppenheimer approximation, vibration of polyatomic molecules. normal
mode of vibration, group frequencies, overtone, hot bands. Raman: Classical and
quantum theories of Raman effect, pure rotational, vibrational and vibrational-
rotational Raman spectra, selection rules, mutual exclusion principle. Resonance
Raman. Molecular Spectroscopy: Energy levels, MO, vibronic transitions, Franck-
Condon principle, electronic spectra of polyatomic molecules. Emission spectra,
radiative and non-radiative decay, internal conversion. Photoelectron spectroscopy.

Text Books:


Reference:

2. Introduction to Molecular Spectroscopy by G. M. Barrow, McGraw Hill

Semester 2

CH-411: Inorganic Reaction Mechanism and Organometallics

Reaction Mechanism: Substitution in octahedral and square planar complexes;
lability, trans-effect, Conjugate base mechanism, racemisation, Electron Transfer
Reactions: inner sphere and outer sphere mechanism, Marcus theory. Inorganic
photochemistry: Photosubstitution and photoredox reactions of chromium, cobalt
and ruthenium compounds, Adamson’s rules. Lanthanides and Actinides: Spectral
and Magnetic Properties, NMR Shift reagents. Organometallic Chemistry: 18-

Text Books:


References:

3. Organometallics by Ch. Elschenbroich, A. Salzer, VCH, 1995, 2nd Ed.

CH-421: Organic Reactions and Mechanisms

Aliphatic Nucleophilic Substitution: The SN₂, S−N¹, mixed S−N¹ and SN² and SET mechanisms. The neighbouring group mechanism. Classical and nonclassical carbocations, phenonium ions, norbornyl system, common carbocation rearrangements. The SN¹ mechanism. Nucleophilic substitution at an allylic, aliphatic trigonal and a vinyl carbon. Reactivity effects of substrate structure, attaching nucleophile, leaving group and reaction medium. Electrophilic Substitution: Aliphatic: Bimolecular mechanisms: SE¹, SE² and SE³. The SE¹ mechanism, electrophilic substitution accompanied by double bond shifts. Effect of substrates, leaving group and the solvent polarity on the reactivity. Aromatic: The arenium ion mechanism, orientation and reactivity, energy profile diagrams. The ortho/para ratio, ipso attack, orientation in other ring systems. Quantitative treatment of reactivity in substrates and electrophiles. Aromatic Nucleophile Substitution: The SNAr, SN¹, benzyne and SRN¹ mechanisms. Reactivity; effect of substrate structure, leaving group and attacking nucleophile. Free Radical

Text Books:


Reference:

1. Modern Synthetic Reactions by H. O. House, W.A. Benjamin, Inc., 1972

**CH – 425: Organic Chemistry Laboratory**

Separation techniques and characterization (t.l.c, column, distillation, crystallization, GC etc.)

Organic synthesis: Representative reaction to be covered

Esterfication and saponification, Oxidation, Reduction, Nucleophilic substitution, Cycloaddition reactions, Grignard reaction, Condensation reactions, Preparation of dyes, Aromatic electrophilic substitution, Heterocyclic synthesis, Solidphase synthesis, Natural product extraction: Solasidine, Caffeine, Nicotine, Peptine, Rosine, Carotenoids, Computational methods of retro-synthetic analysis modeling and calculation

Text Books:

3. Instrumental techniques for Analytical Chemistry by Frank Settle, Printice

Text Books:


References:


Applications of Spectroscopy

Vibrational: Symmetry and shapes of $AB_2$, $AB_3$, $AB_4$, $AB_5$ and $AB_6$, modes of bonding in ambidentate ligands, application of resonance Raman spectroscopy particularly for the study of active sites of metalloproteins. Electron Spin Resonance: Hyperfine coupling, spin polarization for atoms and transition metal
ions, spin-orbit coupling and significance of g-tensor, application of transition metal complexes having one unpaired electron including biological systems and to inorganic free radicals such as \( \text{PH}_4^-, \text{F}_2^- \) and \([\text{BH}_3]^-\).

Nuclear Magnetic Resonance: The contact and pseudo contact shifts, factors affecting nuclear relaxation, some applications including biological systems, an overview of NMR of metal nuclides. Chemical shift, spin-spin interaction, shielding mechanism, complex spin-spin interaction, virtual coupling stereochemistry, hindered rotation, Karplus curve, variation of coupling constant with dihedral angle, nuclear magnetic double resonance, simplification of complex spectra, shift reagent, spin tickling, nuclear overhauser effect (NOE), resonance of other nuclei. 13C NMR: Chemical shift, 13C coupling constants, two-dimensional NMR spectroscopy, NOISY, DEPT, INEPT terminology.

Mössbauer: Basic principles, spectral parameters and spectrum display. Application to the studies of (1) bonding and structures of \( \text{Fe}^{2+} \) and \( \text{Fe}^{3+} \) compounds including those of intermediate spin, (2) \( \text{Sn}^{2+} \) and \( \text{Sn}^{4+} \) compounds – nature of M-L bond, coordination number, structure and (3) detection of oxidation state and inequivalent MB atoms. Electrochemical techniques: CV, polarography, coulometry, amperometry. Thermal Methods: TGA, DSC and DTA

UV-Vis: Woodward rule for conjugated dienes and carbonyl compounds. IR: Characteristic vibrational frequencies of different functional groups, effect of hydrogen bonding and solvent effect on vibrational frequencies, overtones, combination and Fermi resonance bands.

Mass: Instrumentation, Mass spectral fragmentation of organic compounds, McLafferty rearrangement, examples of mass spectral fragmentation of organic compounds with respect to their structure determination.

ORD & CD: Definition, deduction of absolute configuration, octant rule for ketones.

Data Analysis: Uncertainties, errors, mean, standard deviation, least square fit, testing the fit (C2 test, residual etc.). Signal to noise ratio.

Text Books:


References:


**Semester 3**
CH 511: Principles of Bioinorganic Chemistry

Role of alkali and alkaline earth metal ions in biology; Na\(^+\)-K\(^+\) Pump, ionophores and crown ethers. Metal site structure, function. Metal ion transport and storage: Ferritin, Transferrin, Siderophores and metallothionein. Electron Transfer: Cytochromes, Iron-Sulfur Proteins and Copper Proteins. Oxygen transport and storage: Hemoglobin, myoglobin, hemerythrin, hemocyanin. Oxygen activation: Cytochrome P450, Cytochrome c oxidase. Other metal containing enzymes: Catalase, peroxidase, superoxide dismutase, alcohol dehydrogenase, carbonic anhydrase, carboxypeptidase, xanthine oxidase, nitrogense, vitamin B12 coenzyme, photosystem I and II, oxygen evolving center. Various spectroscopic methods used in bioinorganic chemistry: electronic spectra, EPR (emphasis on first row transition metal ions and their spectra), brief description of CD / MCD and multinuclear NMR. Applications of newer methods like EXAFS, XANES and ENDOR in characterization of biological molecules. Use of coordination complexes as models for various enzymes, metalloproteins. Role of hazardous materials such as nitric oxide, cyanide and methyl isocyanate etc. in biological systems.

Text Books:

References:

CH 520: Concepts in Organic Synthesis

Pericyclic Reactions: Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl system. Classification of pericyclic reactions. Woodward-Hoffmann correlation diagrams. FMO and PMO approach. Electrocyclic reaction; conrotatory and disrotatory motions 4n, 4n+2 and allyl systems. Cycloaddition; antrafacial and suprafacial addition, 4n and 4n+2 systems, 2+2 addition of ketenes, 1,3 dipolar cycloadditions and cheleotropic reactions. Sigmatropic Rearrangements; suprafacial and antrafacial shifts of H, sigmatropic shifts involving carbon moieties, 3,3- and 5,5- sigmatropic rearrangements, Claisen, Cope and Aza-Cope rearrangements. Ene reaction. Photochemistry: Quantum yields, intersystem crossing, photosensitization and energy transfer reactions. Photochemistry of olefins and carbonyl compounds, photo oxygenation and photo fragmentation, Photochemistry of aromatic compounds: isomerisation, additions and substitutions. Singlet molecular oxygen reactions. Patterno-Buchi reaction, Di-pimethane rearrangement, Bartons reaction and Photo-Fries

Text

Books:


Reference:


CH 521: Modern Techniques and Scope of Chemical Biology

Chemical biology: definition, history. Peptide and Protein: amino acids, peptides, primary, secondary, tertiary, and quaternary structure of proteins, protein folding. Protein Synthesis: biosynthesis, chemical synthesis, solid phase peptide synthesis, strategy of combinatorial synthesis, combinatorial solid phase synthesis of antibiotics. Lipids: fatty acids, bilayer, lipidation of proteins and peptides, farnesylation of the Ras protein. Insertion of lipidated peptides into model membrane: biological membranes, transport across membranes, model membrane, biophysical properties of lipidated peptides in model membranes, basic concepts of fluorescence and fluorescence markers, synthesis of vesicles containing fluorescence quencher and lipidated peptides. Nucleic acids: base pairing, double helices, DNA replication, genetic information storage, transmission and gene expression, chemical synthesis of oligonucleotides, hybridization with synthetic oligonucleotides. Peptide nuclic acids (PNAs), synthesis of PNAs, doubly labeled PNAs as probes for the detection of point mutations. Use of small molecules to link a protein target to a cellular phenotype and as probes for biological processes.
CH-530: Classical and Statistical Thermodynamics  3  1  0  8


Text Books:
Reference:

CH-535: Physical Chemistry Laboratory 1 0 8 10

Experiments based on
UV - Visible spectroscopy with application
Fluorescence Spectroscopy with application
Infrared Spectroscopy
Solvents effects in spectra
Differential Scanning Calorimetry
High Pressure Liquid Chromatography
Spectroscopy Instrumentation
Cyclic voltametry
Temperature dependence of reaction rates
Enzymetic reaction
LB films / Liposomes
Ion selective electrodes
Semiconductor materials
Optical materials

Text Books:
3. Journal of Chemical Education, ACS: some selected readings and experiments will be offered from this journal.

Semester 4

CH 640 Principles and Applications of Luminescence Spectroscopy 3 1 0 8

Luminescence, a brief history, different kinds of luminescence, electronic transition, transition probability, fluorescence and other de-excitation process, phosphorescence versus non-radiative de-excitation, delayed fluorescence, basic instrumentation of steady-state and time-resolved fluorometer, characteristics of
fluorescence emission, solvent and environmental effects, red-edge effects, effects of intermolecular photophysical processes on emission, static and dynamic quenching, Stern-Volmer kinetics, emission anisotropy, intrinsic and extrinsic probes, chemical sensing probes, probes of analyte recognition, electron transfer probes, energy transfer, energy transfer to multiple acceptor, biochemical applications, pH and CO₂ sensors, protein fluorescence and protein sensors, glucose sensors, novel fluorophores: semiconductor nano particles, lanthanides, metal-ligand complexes, long-wavelength and long-lifetime fluorophores, advanced techniques in fluorescence spectroscopy.

Text Books:


References:


CH 501: Computers in Chemistry 2 0 1 5

Computer programming in FORTRAN. Computer application in Chemistry: Development of small computer codes involving simple formulae in chemistry, such as van der Waals equation, pH titration, kinetics, radioactive decay. Evaluation of lattice energy and ionic radii from experimental data. Linear simultaneous equations to solve secular equations within the Hückel theory. Elementary structural features such as bond lengths, bond angles, dihedral angles etc., of molecules extracted from a database such as Cambridge database.

Use of computer programmes: Execution of linear regression, X-Y plot, numerical integration and differentiation as well as differential equation solution programmes. Monte Carlo and Molecular dynamics. Programmes with data preferably from physical chemistry laboratory.

Text Books:

1. Computational Chemistry by A. C. Norris, John Wiley
Reference:

1. Inside the IBM PC by Peter Norton

CH 615 Advanced Organometallic Chemistry 3-0-1-8


Applications of transition metal complexes to catalysis, organometallics directed towards organicsynthesis.


Text Books:


CH 637: Advance Quantum Chemistry 3 1 0 8


Approximate solutions to the Schroedinger equation: The Variation method (Time independent and Time Dependent), Time independent perturbation theory (non – degenerate and degenerate), Time dependent perturbation theory.


The Hartree-Fock Self-Consistent Field Method: The generation of Optimized orbitals, Koopman’s Theorem (The Physical Significance of Orbital Energies), The electron correlation energy, Density matrix analysis of the Hartree-Fock
Approximation, Natural orbitals, The matrix solution of the Hartree- Fock Equations (Roothaan’s equations).

**Introduction to Molecular Structure:** The Born - Oppenheimer Approximation, Solution of the Nuclear Equation, Molecular Hartree- Fock Calculations.

**Electronic Structure of Linear Molecule:** The MO - LCAO Approximation, The Hydrogen Molecule Ion, H\(_2^+\), The Hydrogen molecule, Molecular Configuration - Interactions, The Valence Bond Method, Molecular Perturbation Calculations.

**Electronic Structure of Non-linear Molecule:** The \(\text{AH}_n\) molecule: Methane, Ammonia and Water, Hybrid Orbitals: The Ethylene and Benzene Molecules.


Text Books:


References:


**CH 628 Advances in Nucleic Acid and Lipid Chemistry**


Text books:

References: