National University

Subject: Chemistry

Syllabus for Four Year B.Sc. Honours Course
Effective from the Session: 2013-2014

Year wise Paper, Marks and Credit distribution

FOURTH YEAR

<table>
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<tr>
<th>Paper Code</th>
<th>Paper Title</th>
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<td>Physical Chemistry-IV</td>
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<tr>
<td>242803</td>
<td>Selected Topics in Organic Chemistry</td>
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<tr>
<td>242805</td>
<td>Selected Topics in Inorganic Chemistry</td>
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<td>242807</td>
<td>Nuclear Chemistry</td>
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<td>242809</td>
<td>Organic Polymers</td>
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<td>242811</td>
<td>Reaction Mechanism</td>
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<td>242813</td>
<td>Separation Techniques</td>
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<td>Chemical Spectroscopy</td>
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<td>Practical Chemistry (Organic)</td>
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## Detailed Syllabus

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<tr>
<td>Paper Title:</td>
<td>Physical Chemistry-IV</td>
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1. **Quantum Chemistry:** Failure of classical mechanics, black body radiation, Planck’s quantum theory, photoelectric effect, Einstein’s explanation of the photoelectric effect, Compton effect, heat capacities of solids, atomic spectra, de-Broglie’s hypothesis, diffraction of electrons, consequences of de Broglie’s concepts, Heisenberg’s uncertainty principle, consequences of the uncertainty relation.

2. **Schrodinger wave equation and it’s solution:** The time-independent Schrodinger wave equation, operators in quantum mechanics, eigenfunctions and eigenvalues, well behaved wave functions, significance of wave functions, postulates of quantum mechanics, applications of quantum mechanics, particle in a one-dimensional box, degeneracy, Schrodinger wave equation for the hydrogen atom, separation of variables, \( \Phi \), \( \Theta \) and \( R \) equations, solutions of the \( \Phi \) and \( \Theta \) equations, the perturbation theory, perturbation treatment of the helium atom ground state, the variation theorem, variation treatment of the ground state of helium.

3. **Statistical Mechanics:** Macroscopic system, configuration, population, weight, Boltzmann distribution, molecular partition function: translational, rotation and vibrational partition functions of molecules, internal energy of a system, Fermi-Dirac and Bose Einstein statistics, evaluation of partition function, calculation of thermodynamic function, Einstein and Debye equation, chemical equilibrium, statistical treatment, evaluation of equilibrium constant.

### Books Recommended:

2. Quantum Chemistry, Donald A McQuarri.

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<tr>
<td>Paper Title:</td>
<td>Selected Topics in Organic Chemistry</td>
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1. **Natural Products**

1.1. **Carbohydrates:** Sources and importance, Classification, structure and configuration of aldoses and ketoses projection formula and conformation, reaction of monosaccharides. Structure and conformation of aldo-hexoses structure of sucrose, maltose and lactose, mutarotation, anomeration, epimerization, determination of ring size, conformation of aldo-hexoses.
1.2. **Alkaloids**: Occurrence and importance Classification, Tests of alkaloids, extraction and purification of alkaloids; general methods of determining the structure, Chemistry of ephedrine, nicotine, papaverine and atropine.

1.3. **Terpenes**: The essential oils; Classification of terpenes; Isoprene and special isoprene rule, isolation, purification and general methods of determining structures of terpenes; Detailed studies of some mono terpenes; i. acyclic-citral, ii. Monocyclic.

1.4. **Amino-acids and Proteins**: Structure, Classification, synthesis, physical and chemical behaviour of amino-acids; Isoelectric point of amino-acids, analysis of amino-acids; structure and synthesis of peptides, general nature and assay of polypeptides and proteins.

1.5. **Urides and Purines**: Isolation and purification of purine bases; Structure and synthesis of uric acids, structures of important derivatives of purines; Adenine, Xanthine, Guanine, Nucleotides; Nucleosides and Nucleic acids.

1.6. **Colouring Matters**: Isolation, purification and structure of anthocyanines, Flavonoids and Carotenoids.

1.7. **Steroids**: Occurrence classification and detection of steroids, Structure elucidation of steroids with reference to β-sitosterol, cholesterol

2. **Medicinal Chemistry**

1. **Synthesis of Some Important Organic Drugs:**

   1.1. **Sulpha Drugs**: Sulphanilamide, Sulphapyridine, Sulphathiazole.

   1.2. **Antimalarials**: Plamaquine, Mepacrine, Chloroquine & Paludrine.

   1.3. **Fever Sinking Drugs**: Paracetamol, Aspirin, Phenacetin.

   2. **Antibiotics**: Penicilin. Steptomycin, Chloromycetin.

Books Recommended:

1. An Introduction to the Chemistry of Carbohydrates, R.D. Guthrie and John Honeyman
2. Carbohydrate Chemistry, Davison.
3. Chromatographic Methods. Stock and Rice
5. Chemistry of Alkaloids Pelletier. Van Nostrand

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| Paper Title: | Selected Topics In Inorganic Chemistry |

1. **Molecular Symmetry and Group Theory**: Symmetry elements and operations, point groups of molecules, groups of very high and low symmetry, use of flow chart to identify a point group, optical activity and dipole moments on the basis of point group symmetry.
2. **Bioinorganic Chemistry:** Essential and non-essential elements, availability of bioelements, deficiency and specificity of bioactive elements, roles of Na\(^+\) and K\(^+\), ion pump, role of calcium in muscle contraction, role of magnesium in photosynthesis, biochemistry of iron, hemoglobin and myoglobin, oxygen transport and storage, oxygen carriers, cytochromes, metalloenzymes, iron-sulfur proteins, nitrogen fixation, vitamin B\(_{12}\).

3. **Non-aqueous Solvents:** Classification of solvents, general properties of ionizing solvents, leveling and differentiating solvents, types of chemical reactions in solvents, measurement of solvent strength, liquid ammonia, ethanol, anhydrous sulfuric acid, liquid SO\(_2\), molten salts as solvents.

4. **Inorganic Polymers:** Concept of inorganic polymers as distinct to organic polymers, classification of inorganic polymers, properties of inorganic polymers, studies of some typical inorganic polymers: (i) phosphazines, (ii) silicones, and (iii) S-N polymers.

5. **Nanochemistry:** Overview of different nanomaterials available, classification, Methods for the synthesis and characterization of nanomaterials, fullerenes and carbon nanotube, applications of nanomaterials.

6. **Metal Clusters:** Introduction, synthesis, structures of metal clusters with pi-acid ligands - polyhedral skeletal electron-pair theory, the capping principle, reactions of metal clusters, applications.

**Books Recommended:**


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<tr>
<td>Paper Title:</td>
<td>Nuclear Chemistry</td>
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1. **The Atomic Nucleus and Its Properties:** Atomic nucleus and its constituents, nuclear radius and nuclear density, nuclear force, mass defect, packing fraction, binding energy, nuclear spin and moments, nuclear potential, concepts of nuclear structure - shell model, nuclear statistics, nuclear stability, nuclidic mass and atomic mass, nuclear mass and energy correlation, classification of nuclides.

2. **Radioactivity and Radioactive Decay Laws:** Radioactivity, units of radioactivity, natural and artificial radioactivity, radioactive decay, kinetics of radioactive decay, half-life and average life, radioactive decay series, radioactive equilibria, comparison between radioactive equilibrium and chemical equilibrium.

3. **Nuclear Reactions:** Nuclear reactions and their comparison with chemical reactions, types of nuclear reactions, conservation laws, energetics of nuclear reactions, nuclear reaction cross-section, excitation function, nuclear reactions mechanisms, nuclear fission and liquid drop model,
fissionability parameters, the mass, charge and kinetic energy distributions in thermal neutron induced fission of $^{235}\text{U}$, practical application of nuclear fission, nuclear fusion, controlled nuclear fusion, importance of nuclear fusion.

4. **Interaction of Radiation with Matter and Detection of Nuclear Radiation:** Modes of interactions, interactions of gamma radiations and charged particles with matters, Bremsstrahlung radiation, Čerenkov radiation, beta backscatter, the Auger process, radiation detection, measurements of radiations with ionization chambers, proportional counter, Geiger Müller counter, NaI(Tl) scintillation detectors.

5. **Nuclear Reactors:** The fission energy, fission cross-sections and threshold, fission neutrons, the reproduction factor, Fermi’s four factor formula, major components of a reactor, the classification of reactors, reactor power, critical size of a thermal reactor, excess reactivity and control, breeder reactors, application of reactors.

6. **Accelerators:** Working principles, basic components and utilization of Van de graaff, tandem Van de graaff, cyclotron and synchrotrons accelerators.

7. **Production and Uses of Radioisotopes:** General principles of production of radioisotopes, radiochemical separation and purification of isotopes, uses of radioisotopes.

8. **Nuclear and Radiochemical Methods of Analysis and their Applications:** Radiotracer, geochronology and radioactive dating, isotope dilution method in chemical analysis, neutron activation analysis of trace elements.

9. **Safety:** Radiation exposure, radiation dose, dose equivalent, quality factor, simple calculation of radiation exposure and radiation dose for γ- and β-rays, radiation hazards, radiation protection and control, radioactive wastes and their management.

**Books Recommended:**


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<td>Paper Title:</td>
<td>Organic Polymers</td>
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1. **Classification of Polymers & Polymerization Process:** Addition (Chain reaction) and Condensation (Step reaction) Polymerizations

2. **Fundamental Concept of the Following Polymer:** Homopolymers and heteropolymers. Low density and high density polymers and their properties. Copolymers; alternating, random, block and graft copolymers. Elastomer, thermoplastic and thermosetting polymers and their properties. Fiber and elastomer.
3. **Mechanism of polymerization:** Redical, cationic and anionic polymerization, and their kinetics, Chain termination, Chain transfer, Chain retardation and chain inhibition.

4. **Co-ordination polymerization:** Fluid-bed process, Ziegler-Natta Catalysis, mechanism of co-ordination polymerization and its kinetics, Metal oxide catalyzed and Olefin polymerizations. Ring opening polymerization.

5. **Configuration of polymers:** Syndiotactic, isotactic, atactic polymers.

6. **Some important polymers:** Production of monomer unit, physical properties and important uses of polythene, polyvinylchloride (PVC), polystyrene, polybutylene, polybutadiene-styrene, neoprene, polymethylmethacrylate, polyacrylonitrile, polyvinylacetate, polyamides: Nylon 6, nylon 66, nylon 11 and nylon 12, silk and wool.

7. **Thermosetting resins:** Phenol-formaldehyde, phenol-urea, melamine-formaldehyde polymers, their preparation and uses. Epoxy resins and polyuranthanes.

**Books Recommended:**

2. Text book of polymer science, F.W. Billmeyer, JR

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<td>Paper Title:</td>
<td>Reaction Mechanism</td>
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1. **Broad concept of the mechanism of the following classes of organic reaction:**

   1.1 **Nucleophilic Substitution at Saturated Carbon:** Mechanism of $S_N1$ and $S_N2$; stereochemistry and kinetics of $S_N1$ and $S_N2$ reactions; broad concept of effect of solvent, effect of structure, effect of attacking reagents and leaving groups, neighbouring group participation, Steric effect. nucleophilic substitution at unsaturated carbon with special reference of Claisen condensation reaction; Aromatic nucleophilic substitution reactions.

   1.2 **Electrophilic substitution Reactions:** Electrophilic substitution reactions at unsaturated carbon including aromatic compounds; nitration, halogenation, sulphonation alkylation and acylation.

   1.3 **Electrophilic addition reactions:** Electrophilic addition to $C=\text{C}$ and $C\equiv\text{C}$ bonds; halogenation, hydrogenation, hydration, hydroxylations, hydorboration, ozonolysis, Diels-Alder reaction, Michael addition.
1.4 **Oxidation-Reduction Reactions:** Wolff-Kishner reduction, Clemmensen reduction, Oppenauer oxidation; reduction with metal hydrides; Rosenmund reduction, Wittig reaction Meerwein-Ponndorf-Verley reduction.

2. **Addition:** Mechanism & stereo chemistry of nucleophilic addition to C=O bond with special reference to Cannizzaro reaction, Aldol condensation, Perkin reaction, Reformatsky reaction, Benzoin condensation, Mannich reaction, Grignard reaction Knoevenagel reaction. 1,3-Dipolar addition and 1,4-addition reactions.

3. **Elimination:** E₁ & E₂ mechanism; stereochemistry and orientation of elimination reactions; competition between elimination and substitution; intramolecular elimination. Ionic elimination, thermal and syn-elimination (Chugaey and related reactions). Detailed treatment of Saytzeff and Hofmann rule of elimination reaction leading to product formations.

4. **Molecular Rearrangements:** Base-catalysed rearrangements, rearrangements involving migration to electron deficient nitrogen and oxygen atoms; aromatic rearrangement passing though “No mechanism pathways” Clasien, Cope and related rearrangements.

5. **Conformational Analysis and its Effect on Reactivity:** Conformational effects on stability and reactivity Courtius-Hammet principle. transannular effects. The concept of 1-strain.

6. **Molecular Orbital Theory:** Phase of an orbital and its role in bonding and antibonding. Huckel molecular orbital theory. LCAO’s theory and M.O’s theory – their shapes and energy states. Illustration with 1,3-butadiene allyl system and 1,3,5-hexatriene.

7. **Orbital Symmetry and Chemical Reactions:** Woodward and Hofmann rules and their applications in thermal and photochemical reactions, electrocyclic reactions, cycloaddition reaction and sigmatropic rearrangements.

**Books Recommended:**

8. Symmetry in organic Molecules, Gilchrist and Storr.
9. Frontier Orbital Theory, I Fleming
10. Organic Reaction Mechanism, E.S. Gould
### Paper Title: Separation Techniques

1. **Solvent Extraction:** Introduction, completeness of extraction, selectivity of extraction, factors favoring solvent extraction, solvent extraction equilibria, batch and continuous extractions, analytical applications.

2. **Chromatographic Methods in General:** Introduction, retention behavior, efficiency, selectivity, resolution, chromatographic theory, measured chromatographic parameters, evaluation methods, classification of chromatography.

3. **Liquid Chromatography:** Introduction, technique of liquid chromatography, various forms of liquid chromatography, ion pair chromatography, principles of ion pair extraction, retention, selectivity, application.

4. **Paper Chromatography:** Principle, types of paper, choice of solvents, sample application, apparatus, location of spots and measurements of R_F value, separation of amino acids by paper chromatography.

5. **Thin Layer Chromatography:** Theories and mechanism of TLC, choice of adsorbents, choice of solvents, detecting reagents, developing chamber, development and detection, superiority of TLC, analytical applications.

6. **Column Chromatography:** Introduction, the column, packing the column, adsorbent, solvents used with columns, separation techniques, identification of compounds, applications.

7. **Ion-Exchange Chromatography:** Ion-exchange resin, types of resins, their structure and properties, factors affecting the ion-exchange-equilibria, eluting solvents, analysis of the elute, application of ion-exchange chromatography.

8. **Gel Chromatography:** Theory of gel chromatography, column, gel preparation, packing of column, advantages of gel chromatography, applications of gel chromatography.

9. **High-Performance Liquid Chromatography:** The HPLC system, particle size and support material, filtration and degassing, HPLC columns, solvent requirements, solvent pumping systems, injection systems, HPLC detectors, advantages of HPLC, effect of temperature in HPLC, applications.

10. **Electrophoresis:** Definition, Types of electrophoretic methods, paper electrophoresis, paper used, electrodes, source of current, location of components, requirements of electrophoretic chambers, sample introduction and detection, applications.

11. **Gas Chromatography:** Principle, GC columns, selection of materials and column design, stationary phases, carrier gas, sample injection system, general properties of detectors, detector types, theory and principle of gas liquid chromatography, factors affecting separation, applications of gas liquid chromatography.
Books Recommended:


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<tr>
<td>Paper Title</td>
<td>Chemical Spectroscopy</td>
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1. **Electromagnetic Radiation**: The nature of electromagnetic radiation; emission and absorption spectra; spectrometers; basic components of dispersive spectrometers, modulation technique; transmittance and absorbance; representation of spectra; spectral peaks, intensities, width and resolution, signal to noise ratio and signal averaging; fourier transform technique and its advantages.

2. **Rotational spectroscopy**: Rotation of molecules and the classification of rotating molecules with radiation; microwave spectrometer; rotational energies of linear rotors; distribution of molecules and rotational spectra centrifugal distortion; symmetric top molecules and their rotational spectra; effect of isotopic substitution; stark effect and its use in microwaves spectrometers; determination of molecular geometry from microwave spectra.

3. **Infrared spectroscopy**: Vibration in molecules; normal modes, harmonic and anharmonic; potential energy diagrams; Morse equation; vibrational energy; dissociation energy of diatomic molecules; population of vibration levels; transition probabilities; fundamental, overtone and hot band transitions; combination and different bands; farmi resonance; vibration – rotation spectra of gaseous molecules; P, Q and R branches: parallel and perpendicular vibrations; infrared spectra of polyatomic molecule; characteristic group vibrations and skeletal vibrations; shifts in group frequencies.

4. **Ultraviolet-visible spectroscopy**: Electronic states of molecules; spectra of simple gaseous diatomic species and their vibrational Paper structure; Frank-condon principle and intensities of spectral lines; dissociation energy; pre-dissociation; spectra of species in condensed phase; various electronic transitions in organic and inorganic species; width of electronic bands; effect of solvent on band width and band position; chromospheres, bathochromic and hypochromic shifts, auxochromes.

5. **Raman spectroscopy**: Raman effect; classical and quantum concept of raman scattering; criterion of raman activity; raman spectrometers. applications of raman spectroscopy.

6. **Principles of Resonance spectroscopy**: Electron spin and nuclear spin; effect of magnetic field on the energies of spinning electrons and nuclei; the larmor precession; Resonance absorption of radiation through spin flipping; relaxation time’s; NMR spectroscopy: electron density at the nucleus, the chemical shift, and scales of chemical shift; the coupling of nuclear spins, the coupling constant; Exchange phenomenon in
chemical analysis by NMR techniques. ESR spectroscopy: The g-factor, hyperfine splitting. determination of electron density from ESR spectroscopic studies.

7. Mass spectroscopy: Basic Principles, ionization techniques, Electron impaci (EI), Chemical ionization (CI), desorption ionization (DI), Fast Atom Bombardment (FAB), molecular ion peak, meta-stable ions, fragmentation process, McLaffery rearrangement, molecular ion identification, interpretation of mass spectra. instrumentation of mass spectrophotometer.

Books Recommended:
1. The structure of Molecules; G.M. Barrow
2. Introduction of Molecular Spectroscopy; G.M. Barrow
3. Fundamental of Molecular Spectroscopy; C.N. Banwell
4. The Infrared Spectra of Complex Molecule; L.J. Bellamy
5. Ultraviolet and Visible Spectroscopy; Rao
6. Molecular Spectroscopy; Rayfmond Chang
7. Spectra of Diatomic Molecule; Hertzberg
8. Physical Chemistry; P.W. Atkins

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<td>Practical Chemistry (Organic)</td>
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1. Multistep organic synthesis: Paracetamol, Diels-Alder adduct etc.

2. Separation and Identification of mixture of organic compounds by chemical and chromatographic method (using TLC/Column chromatography/paper chromatography)

Books Recommended:
1. Qualitative Organic Analysis, A.I. Vogel
2. Quantitative Organic Analysis, A.I. Vogel
4. Identification of Organic Compounds, Shriner and Fuson
5. Chromatographic Methods, Stock and Rice

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<td>Practical Chemistry (Industrial)</td>
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To Perform two Experiments (one from each group) each of 3 hours duration.

A. Inorgano Industrial Chemistry experiments

1. Determination of water hardness: temporary and permanent hardness.
2. Determination of chloride content in water by Hg (II) nitrate method.
3. Determination of dissolved O₂ in water by NaOH-MnSO₄ method
4. Measurement of pH and conductivity of water
5. Determination of Fe content in an iron tablet.
6. Determination of nitrogen by Kjeldahl’s method
7. Determination of total arsenic, As(III) + As(V), in a groundwater sample
8. Determination of calcium in egg shell.
10. Determination of ascorbic in Vitamin-C tablet
11. Determination of iodine in a salt sample.

B. Organo Industrial Chemistry experiments

1. Determination of iodine value of supplied oil sample.
2. Saponification value of oils and fats.
3. Determination of total acid and alkali in a soap sample
4. Determination of free acid and free alkali in soap sample
5. Determination of acid value of fats and oils.
6. Determination of the amount of glucose with the help of Fehling’s solution.
7. Determination of the purity of sugar with the help of Fehling’s solution.
8. Quantitative analysis of Aspirin.

Books Recommended:

1. Qualitative Organic Analysis, A.I. Vogel
2. Quantitative Organic Analysis, A.I. Vogel
3. Chromatographic Methods, Stock and Rice.

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