M.Sc. Chemistry Part- I

The following will be the structure for Revised Syllabus from June 2008 for semester I and Semester II

**Semester – I**

CH – 110  Physical Chemistry – I  
CH – 130  Inorganic Chemistry – I  
CH – 150  Organic reaction mechanism and stereochemistry. 
CH – 107  Physical Chemistry practical (Departmental Course)  
CH – 127  Inorganic Chemistry Practical (Departmental Course)

**Semester – II**

CH – 210  Physical Chemistry II  
CH – 230  Inorganic Chemistry II  
CH – 250  Synthetic organic Chemistry and Spectroscopy.  
CH – 290  General Chemistry (Departmental Course) elective)  
CH – 247  Organic Chemistry practical (Departmental Course)
Structure of
M.Sc. Part – II :- ORGANIC CHEMISTRY

SEMESTER : - III –

1. CH – 350 Organic Reaction Mechanism
2. CH – 351 Spectroscopic Methods in structure Determination
   B. Green Chemistry, Microwave reactions.
4. CH – 353 Pericyclic Reactions, Free radicals and Photo Chemistry.

SEMESTER :- IV –

1. CH – 450 Chemistry Of Natural Products.
2. CH – 451 Synthetic Methods in Organic Chemistry
3. CH – 452 Heterocyclic Chemistry; Chiron Approach; Medicinal
   Chemistry;
   Vitamins, Hormones Antibiotics etc.

Practical Courses:-

1. CH – 347 Ternary Mixture Separation
2. CH – 447 Two Stage Preparations.
3. CH – 448 Project / Preparations
Important Notes

1. Each theory course prescribed for M. Sc. should be covered in 4 periods, each of 60 minutes duration per week per course including lectures, tutorials, seminars etc.

2. Each practical course will require 6 hours of laboratory work per week and the course will be extended over two semesters and will be examined at the end of the year.

3. There should not be more than 10 students in a batch for M. Sc. practical course.

4. For theory course the question paper should include at least 20% weight age for problem solving. Problem solving would include numerical, short answer, long answer questions to test understanding of the subject.

5. Of the 60 lectures in each course about 10 lectures will include tutorials, student seminars and class tests.

6. Two interactive sessions per course per semester must be conducted by concerned teachers.
1) Recapitulation :-

Heat, Work, & Conservation of energy – The basic concepts, the first law, infinitesimal changes, mechanical work, work of compression & expansion, free expansion, Expansion against constant pressure, reversible expansion, Heat :- heat capacity, enthalpy.

State functions & differentials – state functions, Exact & Inexact differential, changes in internal energy, temperature dependence of the internal energy, Temperature dependence of the enthalpy. Work of adiabatic expansion-Irreversible adiabatic expansion, reversible adiabatic expansion.

Ref 1 Page No. 38 to 74 Periods – 02

2) The Second law of Thermodynamics

Measuring the dispersal the entropy, The second law, the definition of entropy, the entropy changes in the system, natural events. Entropy changes in the universe – The enthalpy change when a system is heated, Entropy changes in surroundings, The entropy of phase transition. The entropy of irreversible changes. Concentrating on the system – The Helmoltz & Gibbs function, some remarks on the Helmholtz function, Maximum work, some remarks to Gibbs function 2.4 Evaluating the entropy & Gibbs function, The Third law of Thermodynamics, Third law entropies standard molar Gibbs function.

Ref 1 Page No. 96 to 117. Periods – 05

3) Combining First & Second Law –


Ref 1 Page No. – 121 – 127, 131. Periods – 03
4) **Changes of State** :
Physical Transformation of pure materials. The stability of phases, Phase
equilibrium & phase diagrams, The solid – liquid boundary, The liquid-vapour

Ref. 1  Pages – 137 to 143.  Periods – 03

5) **Changes of State**
Physical transformation of simple mixtures, Partial molar quantities Partial
molar volume, Partial molar Gibbs function, The thermodynamics of mixing – the
Gibbs function of mixing after thermodynamics mixing functions, The chemical
potential of liquid-liquid mixture, colligate properties- The common features, the
elevation of boiling point, The depression of freezing point, solubility, osmosis,
Mixtures of volatile liquid – vapour pressure diagram – The representation of
distillation, azeotropes, immiscible liquids.

6) **Changes of States** –
Chemical reactions, Which way is downhill – The Gibbs function minimum,
Exergonic & endergonic reaction, perfect gas equilibria, A recipe for equilibrium
constants real gas.

Ref 1  Page-161 to 181, Ref.  Page No. 212 to 217,  Periods – 07

**QUANTUM CHEMISTRY**
Historical development of quantum theory principal of quantum mechanics,
wave particle duality, uncertainty principles, Schrödinger equation, operators simple
system – free particle, Particle in a box, Two dimensional Three dimensional box,
Hydrogen like atoms ( no derivation ) atomic orbital.  Periods – 10

**Reference Books** -
5. Physical Chemistry – Thomas Engel, Philip Reid.

Section – II

1. CHEMICAL KINETICS

1. Recapitulation:-

Reaction rate, Rate law & rate constants, The determination of rate law, first order reactions, second order reactions, Half life.

Ref 1 Page – 689 to 697.  
Periods - 02

2. According for rate laws:-

Simple reactions, The temperature dependence of reaction rates, Reaction approaching equilibrium consecutive reactions, The steady state approximations, Pre-equilibira, Unimolecular reactions, Enzyme catalysis – Michaelis Menton mechanism, Lineweaver and Eadie plots, The kinetics of complex reaction, Chain reactions, the structure of chain reactions Explosions, - Fast reactions, flash photolysis, Flow technique, relaxation methods,

Ref. 1  Page -698 to 708,  Ref 1 Page – 714 to 716  Ref1  Page – 720  Ref. 1 Page 729 to 732  
Period – 12

3. Molecular reaction dynamics:-

Collision theory basic calculation, the steric requirement, Diffusion controlled reactions- Classes of reactions, diffusion & reaction, the details of diffusion, Activated complex. The reaction co – ordinate & transition state, the formulation & decay of the activated complex, How to use the Eyring equation. Thermodynamic aspect, reaction between ions, Dynamics of molecular collisions,

Ref 1  Page – 737 to 758.  
Period - 06

2. STATISTICAL THERMODYNAMICS

Thermodynamic probability of a system, the moat probable distribution, the partition function, systems of independent particles, the energy of a system, the separation of partition function, The partition function for translation, The thermodynamic functions for translation, monochromatic gases, Thermodynamic function for rotation, vibration, & Electronic excitation, Rotation, the electronic portion function, Results of statistical Calculation, statistical calculation of equilibrium constant, entropy & probability, Bose-Einstein & Fermi Dirac Statistics.
Ref. 2 Page – 751 to 772.

Ref. 2 Principles of Physical chemistry – S.H. Maron & C.F. Pruton fourth edition
Ref. 3 Chemicals Kinetics, K.J. Laidler ( Tata Mc. Graw Hill) 1998
Ref. 4 Physical Chemistry, T. Engle and P. Reid, (Pearson Education) 2006
Ref. 5 Basic Chemical Thermodynamics, E. Brian Smith (ELBS) 1990
Ref. 6 Statistical Thermodynamics, L.K. Nash.
Ref. 7 Physical Chemistry molecular approach, D. Mcquarie and J. Simom(Viva) 2000.
Section I: MOLECULAR SPECTROSCOPY (30 Lectures)

1. Recapitulation: Width and intensity of spectral transitions, Fourier transform, microwave spectroscopy, rotation spectra of di- and poly-atomic molecules, Stark effect. (5)

2. Infrared spectroscopy: Harmonic and anharmonic oscillator, vibrational spectra of di- and poly-atomic molecules, coarse and fine structure, Nuclear spin effect, application. (7)

3. Raman Spectroscopy: Introduction, Rotational Raman spectra, Vibrational Raman Spectra, polarization of light and Raman effect, structure elucidation from combined Raman and IR spectroscopy, applications in structure elucidation. (6)

4. Electronic spectroscopy of molecules: Born–Oppenheimer approximation, electronic spectra of diatomic molecules, vibrational coarse structure, rotational fine structure dissociation energy and dissociation products, electronic structure of diatomic molecules, molecular photoelectron spectroscopy, application. (8)

5. ESR and Mossbaur spectroscopy applications. (2)

6. Principles of NMR – Chemical applications of PMR in structure elucidation. (2)

References:

SECTION II: NUCLEAR & RADIATION CHEMISTRY (30)


2) Elements of radiation chemistry – Radiation chemistry, interaction of radiation with miller, passage of nucleous through matter, interaction of radiation with matter, Units. for measuring radiation absorption, Radiation dosimetry, Radiolysis of water, free radiation in water Radiolysis, Radiolysis of some aqueous solution. (08)

3) Nuclear Reactor:

   The fission energy, The Natural uranium reactor, the four factor formula- The reproduction factor K, the classification of reactor. Reactor
power, Critical size of thermal reactor, excess reactivity & control, the Breeder reactor, The Indians nuclear energy programme, Reprocessing of spent fuel: Recovery of Uranium & Plutonium, Nuclear waste management, Natural nuclear reactor. (08)

4) Isotopes for nuclear reactors.
   Isotope separation, separation of selected isotopes, Plutonium. (4)

5) Applications of radioactivity :-
   Typical reaction involved in preparation of radioisotopes:
   $^3$H, $^{14}$C, $^{22}$Na, $^{32}$P, $^{35}$S, and $^{137}$I
   General principles of using radioisotopes.
   - Physical constants – Diffusion coefficients, surface area, solubility.
   - Analytical applications- neutron activation analysis, dilution analysis, radiometric titration.
   - Industrial applications – Radiation gauging, friction and wear out, gamma radiography.

Reference Books.
A) Conductometry:
   i) Hydrolysis of NH₄Cl or CH₃COONa or aniline hydrochloride.
   ii) Determination of λ₀ or λα and dissociation constant of acetic acid.
   iii) Hydrolysis of ethylacetate by NaOH.
   iv) Determination of ..G, ..H, and ..S of Silver Benzoate by conductometry.

B) Potentiometry:
   1. Stability Constant of a complex ion.
   2. Solubility of a sparingly soluble salt.
   3. To determine the ionic product of H₂O
   4. Estimation of halide in mixture.

C) pH metry:
   1. Determination of the acid and base dissociation constant of an amino acid and hence the isoelectric point of the acid.

D) Polarography
   1. Determination of half wave potential E 1/2 and unknown concentration of an ion.
   2. Amperometric titration of Pb(NO₃)₂ with K₂Cr₂O₇

E) Colorimetric :
   1. Analysis of a binary mixture.
   2. Copper EDTA photometric titration.

F) Radioactivity:
   1. Estimation of Mn in tea leaves by NAA
   3. Determination of Emax of beta radiation and absorption coefficients in Al.
G) Chemical Kinetics:
   1. Kinetic decomposition of diacetone alcohol by dilatometry.
   2. Determination of an order of a reaction.
   3. Bronsted primary salt effect.

H) Non-Instrumental :-
   1) Freundlich and Longmuir isotherms for adsorption of acetic acid on active charcoal
   2) Statistical treatment of experimental data
   3) Molecular weight by steam distillation.
   4) Glycerol radius by viscosity.
   5) Partial Molar Volume (Polynometry) Determination of the densities of a series of solutions and to calculate the molar volumes of the components. Each candidate should perform a minimum of 18 experiments with at least one experiment form each technique.

I) Surface area analysis by BET method e.g. industrial pigment

References:-

1. Practical physical chemistry, A. Findary, T.A. Kitchner (Longmans, Green and Co.)
3. Senior Practical Physical Chemistry, B.D. Khosla and V.S. Garg (R. Chand and Co., Delhi.)
A. Symmetry & Stereochemistry (30L)

<table>
<thead>
<tr>
<th></th>
<th>Definitions and theorems of group theory, subgroups, Classes</th>
<th>2L</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>Molecular symmetry and symmetry groups – symmetry elements and operations. Symmetry planes, reflections, inversion centre, proper/improper axes of rotation, products of symmetry operations, equivalent symmetry elements and atoms, symmetry elements and optical isomerism, symmetry point groups, classes of symmetry operations, classification of molecular point groups.</td>
<td>2L</td>
</tr>
<tr>
<td>3</td>
<td>Representations of groups Great orthogonality theorem, character tables, properties of characters of representations. (No mathematical part.)</td>
<td>10L</td>
</tr>
<tr>
<td>4</td>
<td>Group theory and quantum mechanics, Wave function as basis for irreducible representations.</td>
<td>2L</td>
</tr>
<tr>
<td>5</td>
<td>Symmetry Adapted Linear Combinations (SALC) – Projection operators and their use of construct SALC</td>
<td>4L</td>
</tr>
<tr>
<td>6</td>
<td>Molecular Orbital Theory Transformation properties of atomic orbital, MO’s for Sigma bonding ABₙ molecules, tetrahedral AB₄ case.</td>
<td>2L</td>
</tr>
<tr>
<td>7</td>
<td>Crystallographic Symmetry. Unit cell, screw axis, glide plane on unit cell, crystal lattice, space lattice, stereographic projectors. Examples on crystallographic planes, cubic planes, Miller indices, Bravais lattices.</td>
<td>6L</td>
</tr>
</tbody>
</table>
B. Chemistry of Main group Elements

<table>
<thead>
<tr>
<th>1</th>
<th>Hydrogen &amp; its compounds: Hydrides Classification, e deficient, e precise &amp; e rich hydrides PH₃,SbH₃, AsH₃, Selenides, Tellurides.</th>
<th>(3L)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>Alkali &amp; alkaline earth metals Solutions in non-aqueous Media. Application of crown ethers in extraction of alkali &amp; alkaline earth metals.</td>
<td>(2L)</td>
</tr>
<tr>
<td>3</td>
<td>Organometallic compounds of Li, Mg, Be, Ca, Na Synthesis, properties, uses &amp; structures.</td>
<td>(3L)</td>
</tr>
<tr>
<td>4</td>
<td>Boron group Boron Hydrides, preparation, structure &amp; bonding with reference to LUMO, HOMO, interconversion of lower &amp; higher boranes, Metalloboranes, Carboranes.</td>
<td>(4L)</td>
</tr>
<tr>
<td>5</td>
<td>Carbon group Allotropes of Carbon, C₆₀ and compounds (fullerenes), Intercalation compounds of Graphite, Carbon nanotubes, synthesis, Properties, structure- single walled, Multiwalled, applications, classification of organometallic compounds. Organometallic compounds of B, Si, Sn, Pb, Ga,As, Sb, Bi. Structures, Synthesis, Reactions.</td>
<td>(8L)</td>
</tr>
<tr>
<td>6</td>
<td>Nitrogen group Nitrogen activation, Boron nitride, Oxidation states of nitrogen &amp; their interconversion PN &amp; SN compounds Nos, &amp; their redox chemistry.</td>
<td>(3L)</td>
</tr>
<tr>
<td>7</td>
<td>Oxygen group Metal selenides &amp; tellurides, oxyacids &amp; oxoanions of S &amp; N. Ring, Cage and Cluster compounds of P- block elements. Silicates, including Zeolites</td>
<td>(2L)</td>
</tr>
<tr>
<td>8</td>
<td>Halogen group Interhalogens, Pseudohalogen, synthesis, properties &amp; applications, structure, oxyacids &amp; oxoanions of Halogens Bonding.</td>
<td>(3L)</td>
</tr>
<tr>
<td>9</td>
<td>Noble gases Synthesis, properties, uses, structure &amp; bonding with respect to VSEPR.</td>
<td>(2L)</td>
</tr>
</tbody>
</table>
Text Books:

Reference Books:
CH – 127 : INORGANIC CHEMISTRY PRACTICALS.

1. Ore Analysis: At least two of the following:
   a. Determination of Silica and Manganese in pyrolusite
   b. Determination of Copper and iron from chalcopyrite.
   c. Determination of iron from hematite.

2. Alloy Analysis (At least two of the following)
   a. Determination of tin & lead from solder.
   b. Determination of iron & chromium from mild steel.
   c. Determination of copper and nickel from cupronickel.

3. Inorganic Synthesis and Purity determination (any five)
   a. Cis/trans potassium di-aquo di-oxalato chromate (III)
   b. Chloro penta-ammino cobalt (III) chloride
   c. Nitro penta-ammino cobalt (III) chloride
   e. Tris, 2-4 pentanedionato cobalt (III)trihydrate
   f. Potassium tri-oxalato aluminate
   g. Reinecke’s salt.

4. Nickel complexes; Preparation of [Ni(en)₃] S₂O₃, [Ni(H₂O)₆] Cl₂, [Ni(NH₃)₆] Cl₂ and studying their absorption spectra.

5. Ion – exchange chromatography; Separation & estimation of (Zn²⁺ / Cd²⁺) & (Zn²⁺ / Mg²⁺) in mixtures using Amberlite IRA 400 anion exchanger.

6. Instrumental methods of analysis.
   a. Colorimetry:
      i. Simultaneous determination of Cr. & Mn.
      ii. Determination of Keq of M – L systems such as
         Fe (III) – Salicylic acid
         Fe(III) – Sulphosalicylic acid
         Fe(III) – β – resorclic acid by Job’s & Mole ratio method.
      iii. Determination of iron by solvent extraction techniques in a mixture of Fe³⁺, AL⁺³, & Fe⁺³ + Ni⁺³ using 8 - hydroxyquinoline reagent.
b. Conductometry.
   Verification of Debye Huckle theory of ionic conductance for strong electrolytes KCl, BaCl₂, K₂SO₄, K₃[Fe(CN)₆]

c. Table work; (any one)
   i. Analysis of Electronic Spectra of transition metal complexes at least for one system [dⁿ (Oh) or (Td)] and calculation of Crystal Field parameters, interelectronic repulsion parameter and bonding parameter.
   ii. Data analysis, error analysis, lest squares method Plot of Born Maeyer to determine for 1 : 1 type molecule to determine inter nuclear separation. Characterization of metal ligand bonding using IR spectroscopy.

7. Synthesis and Characterisation of nano materials: Quantur dots (cds)

Reference Books:
2) Electronic Spectroscopy by A.B. P. Lever.
3) Inorganic Synthesis (Vol. Series)
4) Practical Manual made By Department of Chemistry, University of Pune.
A. Coordination Chemistry. (30L)

<table>
<thead>
<tr>
<th></th>
<th>Concept &amp; Scope of Ligand Fields</th>
<th>(2L)</th>
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<tbody>
<tr>
<td>2</td>
<td>Energy levels of transition metal ions, free ion terms, term wave functions, spin-orbits coupling.</td>
<td>(6L)</td>
</tr>
<tr>
<td>3</td>
<td>Effect of ligand field on energy levels of transition metal ions, weak cubic ligand field effect on Russell-Saunders terms, strong field effect, correlation diagrams, Tanabe-Sugano Diagrams, Spin-Pairing energies.</td>
<td>(8L)</td>
</tr>
<tr>
<td>4</td>
<td>Electronic spectra of complexes- band intensities, band energies, band width &amp; shapes, spectra of 1st, 2nd &amp; 3rd row ions and rare earth ion complexes, spectrochemical &amp; nephlauxetic series, charge transfer &amp; luminescence, spectra, calculations of Dq, B, β parameters.</td>
<td>(10L)</td>
</tr>
<tr>
<td>5</td>
<td>Magnetic properties of complexes-paramagnetism 1st &amp; 2nd Ordered Zeeman effect, quenching of orbital angular momentum by Ligand fields, Magnetic properties of A, E &amp; T ground terms in complexes, spin free spin paired equilibria</td>
<td>(4L)</td>
</tr>
</tbody>
</table>

B. Bioinorganic chemistry (30L)

<table>
<thead>
<tr>
<th></th>
<th>Overviews of Bioinorganic Chemistry</th>
<th>(2L)</th>
</tr>
</thead>
<tbody>
<tr>
<td>7</td>
<td>Principles of Coordination Chemistry related to Bioinorganic – Protein, Nucleic acids and other metal binding biomolecules.</td>
<td>(9L)</td>
</tr>
<tr>
<td>8</td>
<td>Choice, uptake and assembly of metal containing units in Biology</td>
<td>(7L)</td>
</tr>
<tr>
<td>9</td>
<td>Control and utilization of metal ion concentration in cells.</td>
<td>(8L)</td>
</tr>
<tr>
<td>10</td>
<td>Binging of metal ions and complexes to bimolecular active centers.</td>
<td>(4L)</td>
</tr>
</tbody>
</table>
Text Books:


Reference Books:

## CH- 290 : GENERAL CHEMISTRY
### DEPARTMENTAL COURSE
### ANY TWO PARTS

### PART A

Modern Separation Methods & Hyphenated Techniques: (30L)

<table>
<thead>
<tr>
<th></th>
<th>Description</th>
<th>Duration</th>
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<tbody>
<tr>
<td>1</td>
<td><strong>Gas Chromatography:</strong> Gas chromatography theory and Instrumentation, Column types, Solid/ Liquid Stationary Phases, Column Switching techniques, Basic and Specialized detectors, elemental detection, chiral separations, pyrolysis gas chromatography, High temperature techniques. Application (Clinical, petrochemical etc.) and problems.</td>
<td>(8L)</td>
</tr>
<tr>
<td>2</td>
<td><strong>High performance Liquid Chromatography methods:</strong> HPLC theory and instrumentation, Adsorption chromatography, Liquid-Liquid partition techniques, Microbore and capillary chromatography, Affinity techniques, Size exclusion, ion pair separations, Chiral and Isotope separations, Applications and problems.</td>
<td>(8L)</td>
</tr>
<tr>
<td>3</td>
<td><strong>Ion Chromatography</strong></td>
<td>(2L)</td>
</tr>
<tr>
<td>4</td>
<td><strong>Electrophoresis</strong> : Separation by Adsorption- Affinity techniques, Affinity elution from Ion exchangers and other Adsorbents, Pseudo affinity adsorbents polycrylamide gel electrophorsis, Isoelectric focussing Isotachophoresis, Two dimensional gel electrophoresis, Capillary electrophoresis in rotation- stabilized media, Electrophoresis in stabilized salts, Applications in Nuclei acids, Clinical and capillary zone electrophoresis of carbohydrates.</td>
<td>(6L)</td>
</tr>
<tr>
<td>5</td>
<td><strong>Hyphenated Techniques</strong>&lt;br&gt;Mass spectrometry principle, Instrumentation, Ionization methods – EL, CI, FAB, arc &amp; spark, photoionization, thermal ionization, FI* &amp; FD, laser induced, Photoelectric ionization, SIMS, Mass analyzers – Magnetic, Double focussing, Time of flight, Quadrupolar,Ion cyclotron resonance analyzer. Coupled techniques, GC FTIR, GC-MS (Use of stable isotopes) HPLC-MS.</td>
<td>(6L)</td>
</tr>
</tbody>
</table>
**Text Books:**


**Reference Books**

1. Practical Aspects of Gas chromatography/ Mass spectrometry.


## Part B

Bimolecular: (30L)

<p>| | | |</p>
<table>
<thead>
<tr>
<th></th>
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</table>
| 1 | Cell Structure and function  
Prokaryotes & Eukaryotes membrane & cell structure, subcellular components; nucleus, Mitochondria, Endoplasmic reticulum, Golgi apparatus, Lysosomes, peroxisomes. | (4L) |
| 2 | Water | (2L) |
| 3 | Proteins  
Introduction, Amino acids, Classification of amino acids, physico-chemical properties, reactions with different reagents, Essential & nonessential amino acids. Peptides, end terminal analysis, Primary secondary, tertiary and quaternary structures of Proteins Helix, sheets, super secondary structure, triple helix structures, globular and fibrous proteins. | (8L) |
| 4 | Carbohydrates: Introduction, Classification, structures, stereochemical properties and functions. Derivatives of monosaccharides and their functions. | (5L) |
| 5 | Lipids: Classification, functions. Membrane structure, its organization & functions. | (4L) |
| 6 | Nucleic acids: DNA & RNA types, structure and function. Super coiling of DNA Central dogma, physicochemical properties. | (3L) |
| 7 | Vitamins: Structure, biochemical functions & deficiency disorders. | (4L) |

### Text Book:


### References:

1. Biochemistry (5th edn.) Lubert Stryer.
Part – C
Concepts of Analytical Chemistry:

1. Methods of Analytical Chemistry- Introduction, general analytical process, methods of analytical determination. (4L)

2. Error in chemical analysis – Errors & precision, classification of errors, determinate errors, determination of accuracy of quantitative analytical methods, accuracy sought. (6L)

3. Accuracy & precision – The test of statistics precision, averages, study of an analytical procedure, sampling errors, presentation of results. (6L)

4. Principles & Methods of sampling- Introduction, theory of sampling, pit falls is sampling, technique of sampling gases, liquids and solids, transmission and storage of samples, sources specific sampling information. (8L)

5. Use of Computer programs:
   Linear regression, XY Plots, numerical integration & differentiation, operating with packages such as PCMODEL, WINMOPAC Word processing, Use of MSWORD, Power point & Excel in chemistry, Use of Internet. (6L)

Text Books:


Reference Books:

1. Computational Chemistry , G.Grant and W.Richards, Oxford University press.

Part D : Chemical Mathematics
Part E – Industrial Methods of Analysis.
Part F Computers for chemists.

Note : Syllabus for above said Part- D, Part- E & Part – F is same as the old syllabus.
1. Nature of Bonding in Organic Molecules. (12 lectures)
   A. Delocalized chemical bonding – Conjugation, cross conjugation, resonance, hyper conjugation, tautomerism, inductive Resonance effects.
   B. Acidity and Basicity.
   C. Introduction to aromaticity in Benzenoid and non-Benzenoid compounds, alternant and non-alternant hydrocarbon, Hückel Rule. Bonds weaker than covalent – addition compounds, Crwon ether complexes and Cryptands inclusion compounds, cyclodextrins, Catenanes, rotaxanes and bonding in Fullerenes.
   Ref. 5 (Page No. 26 to 74 and 260 to 272.)

2. Stereochemistry (12 Lectures)
   Ref. 5 (Page No. 94 to 115 and 125 to 130).

3. Aliphatic Nucleophilic Substitution (12 Lectures)
   The SN2, SN1, mixed SN1 and SN2 and SET mechanism. The neighboring group mechanism, The Neighbouring group participation by π & σ bonds, anchimeric assistance, classical and non classical carbocations, phenonium ions, norbornyl syste, carbocation rearrangements in neighboring group participation. The SNi mechanism. Nucleophile Substitution at an allylic, aliphatic trigonal and vinylic carbon. Reactivity effects of structure, attacking Nucleophile, leaving group and reaction Medium Phase transfer catalyst, ambident nucleophile and regioselectivity.
   Ref 5 (Page No. 293 to 369)

4. Addition to Carbon – Carbon Multiple bonds (6 lectures)
   Mechanistic and Stereo chemical aspects of addition reactions involving electrophiles, nucleophiles and Free radicals, Regio and Chemo selectivity, Orientation and reactivity, Michael reaction.
   Ref. 1 (Page no. 167 – 210.)

5. Aromatic Electrophilic Substitution (8 Lectures)
   The arenium ion mechanism, orientation and reactivity, energy profile diagram, The ortho/para ratio ipso attack, orientation in other ring systems, Naphthalene, Anthracene, Six and five membered heterocycles, Diazonium coupling Vilsmeier reaction, Gattermann – Koch reaction, etc.
   Ref. 5 (page no. 501 to 517 and 520 to 545)
6. Aromatic Nucleophilic Substitution (4 Lectures)
   the $S_N2Ar$, $S_N1$ Benzyne & $S_NR1$, Mechanisms, Reactivity effect of substrate structure, leaving group and attacking nucleophile.

   Ref. 5 (Page No. 641 to 653)

7. Elimination reactions (6 Lectures):
   E2, E1, E1cb Mechanisms, Orientation, stereochemistry in elimination, reactivity effect of structure attacking and leaving groups, competition between substitution & elimination, syn eliminations.

   Ref. 5 (relevant pages)

CH – 250: SYNTHETIC ORGANIC CHEMISTRY AND SPECTROSCOPY

1. Oxidation and Reduction (12 Lectures)
   CrO$_3$ (Jones reagent) PDC, PCC, KMnO$_4$, MnO$_2$, Swern, SeO$_2$, Pb (OAc)$_4$, Pd/C, OsO$_4$, mCPBA, O$_3$, NaIO$_4$, HIO$_4$, R$_3$SiH, Bu$_3$SnH, Boranes & Hydroboration reactions, MVP, H$_2$/catalyst, Wilkinson’s catalyst, NaCNBH$_3$, NH$_2$NH$_2$, DIBAL, etc.

   Ref. 1, 2, 10 (relevant pages)

2. Rearrangements (10 Lectures)
   a. Reactive intermediate, Carbocations, carbanions, carbenes, nitrenes

   Ref 3 (page no. 618 to 660)

3. Phosphorous, Nitrogen and Sulphur Ylids and stereochemistry of compounds containing Phosphorous, Sulfur and Nitrogen (4 Lectures)

   Ref. 1, 4 (relevant pages)

4. Addition to Carbon – Hetero Multiple bonds (6 Lectures)
   Addition of Grignard Reagent, Organo Zinc, Organo Copper, and Organo lithium reagents to Carbonyl and unsaturated Carbonyl compounds.

   Ref. 1 (Page No. 376 -394) and (Page No. 615 to 664)
   Ref. 5 (page no. 920 – 936)

5. Conformation of acyclic molecules and shape of six membered rings (6 Lectures)

   Ref. 11 (Page No. 124 to 139 and 204 to 215)
6. Spectroscopy (22 Lectures)
   
   Ref 6, 7 (relevant pages)
   
   Ref. 8 (relevant pages)
   
   c. NMR.: Elementary ideas of NMR Integration, Chemical shifts. Factors affecting, Chemical shifts, Coupling (First order, analysis), Instrumentation & recording of spectra.
   Ref. 6, 9, 13 (relevant pages)
   
   d. Problems in U.V., I.R. and N.M.R.
   Ref. 13
   
References:
8. J. Bellamy, Infrared spectra of Complex molecules.
11. Eliel, Stereochemistry.
13. Pavia Spectroscopy of Organic Compounds
CH – 247 : ORGANIC CHEMISTRY PRACTICALS

1. Techniques:
   Crystallization, fractional crystallization, fractional distillation, vacuum distillation, sublimation, steam distillation, column chromatography, thin layer chromatography (purity would be checked by m.p. and mixed m.p.)

2. Preparation of derivatives.
   Oxime, 2,4 – DNP, acetyl, benzoyl, semicarbazide and aryloxyacetic acid, Anilide, Amide.

   Single Stage (Any Four)
   i) Cyclohexanone to adipic acid.
   ii) Benzaldehyde to dibenzylidene acetone
   iii) Benzaldehyde to cinnamic acid
   iv) P – amino benzoic acid to p-chlorobenzoic acid
   v) 4 – Chlorobenzaldehyde to 4 – Chlorobenzoic acid + -chlorobenzyl alcohol (Cannizzaro reaction)
   vi) Benzene to β – benzoyl propionic acid (Friedel Craft reaction)
   vii) N, N, Dimethylaniline to 4 – Formyl – N, N – Dimethylaniline.
   viii) Benzophenone to Benzpinacol.

4. Double Stage: (Any four)
   i) Phthallic anhydride – Phthallimide – Anthranilic acid.
   ii) Acetophenone – Oxime – Acetanillide.
   iii) Phthalic anhydride – o – benzoyl benzoic acid anthraquinone.
   iv) Chlorobenzene – 2, 4 – dinitrochlorobenzene – 2,4-dinitrophenol.
   v) Benzoin – Benzil – Benzilic Acid

5. Use of Computer - Chem Draw Chem-Sketch, ISI – Draw:
   Draw the structure of simple aliphatic, aromatic, heterocyclic compounds with different subsistent. Get the correct IUPAC name and predict the H1NMR signals.

Ref. 14 (Relevant pages)

- Pattern of practical examination
  Q. 1 Preparation (Single Stage) or Derivative 30 marks
  Q. 2. Techniques : Column or TLC or Steam Distillation 30 marks
  Q. 3 Assignment on computer 10 marks