

# Syllabus of M.Sc. Part-I, Chemistry (D.D.E)

New-Syllabus (From-session: 2014-15)

## A.Theory:

400 Marks

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|---------------|-----|
| 1. Paper-I:   | 100 |
| 2. Paper-II:  | 100 |
| 3. Paper-III: | 100 |
| 4. Paper-IV:  | 100 |

## B. Practical:

200 Marks

- |                |    |
|----------------|----|
| 1. Physical:   | 50 |
| 2. Organic:    | 50 |
| 3. Inorganic:  | 50 |
| 4. Industrial: | 25 |
| 5. Computer:   | 25 |

C. Examination Hour: 4 hrs (Theory papers), 6 hrs (Physical, Organic, Inorganic), 3 hrs (Industrial), 2 hrs (computer)

Paper-1  
Physical Chemistry  
F.M.-100

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- Module-1: Element of Calculus, Extremum Principle, Constrained Extermization, Powerer Series, Fourier Transformation, Vectors and vector Space.
- Module-2: Quantum Mechanics-1:  
Postulates and their analysis, Properties of Operators and Commutators, Angular momentum Operator, Equation of Motion, Stationary States, Ehrenfest's Theorems, Barrier Problems
- Module-3: Quantum Mechanics-2:  
Bound States, Box with infinite and finite Walls, Harmonic Oscillator(Wave function and Operator method), Hydrogen atom problem, Cartesian and Polar Co-ordinates, Center of Mass and Relative Co-ordinate, Spherical Harmonics, Real and Complex Orbital, Roll of Constant of Motion
- Module-4: Electrochemistry-1:  
Debye Huckel Theory, Its modification and Extention, Mean ionic activity Co-efficient, Ion association and precise determination of Dissociation constants of weak electrolite by method of emf and conductance measurement, ion solvent interaction and solvation number
- Module-5: Electrochemistry-2:  
Non stationary process in electrolytic solution, Onsagar conduction equation, Effect of high electric field and frequency on ion conductance, Overvoltage , polarography, Amperometric titration, Basic principle of cyclic voltametry and coulometry, polyelectrolyte
- Module-6: Thermodynamics:  
Maxwell's relations, thermodynamic equation of state, Partial molar quantities, Thermodynamics of mixing, Activity and fugacity applications ion real systems, Nerst heat theorem, Third Law of thermogynamics, Distribution of molecular velocities, Principal of equipartition of energy, Collission frequency, Thermal conductivity, General diffusion expression and Fick's laws, General features of transport matter(Diffusion), Thermal energy (Thermal conductivity and momentum viscosity)

- Module-7: Statistical Mechanics:  
Phase cell, Macrostate, Thermodynamical probability and entropy, Maxwell-Boltzman, Bose-Einstein and fermi-Dirac Statistics, Partition functions of diatoms(Translational, rotational, vibrational and electronic)
- Module-8: Chemical Kinetics & Surface Chemistry:  
Principle of detailed balancing(Simple idea only), Opposing and consequitive reactions, flow and relaxation methods of measurements of reaction rates, flash photolysis, kinetics of fast reaction, Homogeneous and heterogeneous catalysis, enzyme catalysis and inhibition, auto catalysis, oscillatory reactions(general information only), redox reactions, Preliminary idea of Transition state theory.  
Young-Laplace equation, surface (Interface) thermodynamics, Adsorption isotherms (Langmuir and BET with derivation), Surfactants, micelles and emulsion and their applications.
- Module-9: Molecular Spectroscopy-1:  
General Introduction, Nature of Electro magnetic radiation, Shapes and width of spectral lines, intensity of spectral lines, Fourier transform.  
Microwave Spectroscopy: Moment of Inertia and classification of molecules, Diatomic molecule as rigid rotator, non rigid rotator, Hyperfine structure, Stark Effect and determination of Dipole moment,  
Infrared Spectroscopy: Vibrational spectra of diatomic molecules, Harmonic Oscillator model, Anharmonic oscillator model, Rotational Vibrational spectra of diatomic molecules.
- Module-10: Molecular Spectroscopy-2:  
Raman Spectroscopy: Introduction, Classical theory of Raman scattering, Q.M. Picture of a Raman Scattering, Characteristic parameter of Raman lines, Pure Rotational and vibrational Raman spectra, Basic Principles of Raman spectrometer, Application of Raman Spectroscopy  
Electronic Spectroscopy: MO and LCAO (Term Symbol (Linear Molecules) of Molecular States, Electronic energy state of polyatomic molecules, Radiative and Nonradiative process, Franck-Condon principle.

Paper-II  
Organic Chemistry  
F.M.-100

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- Module-1: Pericyclic Reaction-1  
Pericyclic reactions-characteristics features, conservation of orbital symmetry MO of different polyenes, electrocyclic, cycloaddition, sigmatropic reactions, rationalization of different examples with the basis of frontier orbital interaction, Woodward-Hoffmann symmetry rules for pericyclic reactions, exceptions to symmetry rules, correlation diagram of different pericyclic reactions, problem relating to these reactions
- Module-2: Pericyclic Reaction-2  
Perturbation molecular orbital theory (PMO), energy diagram of ethylene and butadiene system with different substituents and study of their cycloaddition reaction, orbital coefficient and diagram of polyene systems with various substitutions. Regioselectivity and site selectivity, secondary interactions in pericyclic reactions cheletropic reactions, Problems relating to these reactions
- Module-3: Organic Transformation/reagent Chemistry/Synthesis-I  
Cation-olefin cyclization reaction: application to the synthesis of triterpenes: biogenetic isoprene rule: monocyclic, bicyclic, tricyclic and pentacyclic ring systems, Fragmentation reaction, Remote functionalization: biomimetic reactions/template effect, examples functional groups interconversion, Multicomponent reactions: Definition, early examples, Passerine reaction, Ugi reaction, Olefin metathesis reaction: Definition, Ring closing metathesis reaction, examples. Phase transfer catalysis,
- Module-4: Organic Transformation/reagent Chemistry/Synthesis-II  
Oxidation reactions: Hydroxylation reagents, use of peroxy acids, Woodward Prevost hydroxylation, Sharpless asymmetric epoxidation, AD-mix, Transformation of epoxides, Organophosphorus reagents, organo sulfur reagents, organo boranes, organo silanes, organostannanes, metal hydrides, Birch reduction, Beyer Villiger reactions, chichibabin reaction, Merrifield resin: solid phase synthesis, Retro synthetic analysis: disconnection approach, examples to illustrate disconnection approach in organic synthesis.
- Module-5: Natural Products-Terpenoids:  
Terpenoids: Isoprene rules, acyclic monoterpenoids, central geraniol neral, linalool monocyclic monoterpenoids: terpineol, structure elucidation, synthesis and biogenesis. Higher terpenoids: P sesquidi-, sester-, tri-, tetra-terpenoids.

- Module-6: Natural Products-Alkaloids  
Alkaloids: Phenyl ethyl amine, quinine, nicotine, peptides, nucleoside and nucleotide structure, synthesis and biogenesis
- Module-7: Stereochemistry-1  
Different projection formula and their interconversions, Conformational and configurational enantiomers, stereochemical nomenclature (E,Z), chiral center, chiral plane, helicity, threo-erythro, pref-parf, chiral simplex. Stereogenicity and chirotopicity. Symmetry and molecular chirality. Stereochemical features: cyclohexane and its derivative conformation and physical properties. Computation of stereoisomers of different systems. Conformation and reactivity of diastereomers 2-, 3-, and 4-Alkyl ketone effects
- Module-8: Stereochemistry-2  
Prochirality and Prostereoisomerism. Topicity and Reactivity. Asymmetric synthesis: Addition of a chiral reagents to chiral ketones and aldehyde, models of stereochemical control: Cram, Felkin and Karabatsos. Atropisomerism Molecular rearrangements with neighbouring group participations. Stereospecific and stereoselective reactions. Sharpless Epoxidation
- Module-9: Heterocyclic  
Heterocyclic: Monocyclic and bicyclic heterocyclic having one and two hetero atoms: synthesis, structure and reactivity.
- Module-10: Spectroscopy  
Application of spectroscopy ( $^1\text{H}$  NMR, UV, IR) in structure determination of organic compounds, Aromaticity, Anti aromaticity, Homoaromaticity, Annulene systems

Module-1: Symmetry and Group theory-I

Groups and their properties-the concept of groups; subgroups classes and their related theorems; commutative (abelian) groups and cyclic groups and their examples; group multiplication tables and the rearrangement theorem. Symmetry elements and operations, products of symmetry operations, equivalent symmetry elements and equivalent atoms, symmetry in platonic solids, identification of point groups, symmetry of  $C_{60}$  fullerenes, Crystallographic symmetry, Hermann-Mauguin notation, optical activity and dipole moment on the basis of point group symmetry; similarity transformation and the invariance of characters; block diagonalisation; direct product of matrices and their characters etc. Matrix representation of symmetry operation, Characters of symmetry operations in a representation, invariance of character under similarity transformation, the row/column orthogonality of character, reducible and irreducible representation, the great 'Orthogonality Theorem' and its corollaries

Module-2: Symmetry and Group theory-II

Character table ( $C_{2v}$ ,  $C_{3v}$ ,  $C_{4v}$ ,  $D_4$ ) representation for cyclic groups wave function as bases for irreducible representations, the standard reduction formula; the direct product representation and its decomposition, identifying nonzero matrix element, spectral transition probabilities, allowedness – forbiddenness of  $n-\pi^*$  and  $\pi-\pi^*$  symmetry of normal modes, normal mode analysis, selection rule for IR and Raman transitions. Projection operator (without derivation), use of the projection operator to form symmetry adapted linear combination (SALC) of simple system

Module-3: Chemical Bonding

Ionic bonds, covalent bonds, metallic bonds, hydrogen bonds, and Van der Waals forces. Variation method, LCAO method, Molecular Orbital Theory of  $H_2^+$ ,  $H_2$ , homo and hetero diatomic, triatomic and polyatomic (including  $T_d$ ,  $O_h$  and  $D_{4h}$  coordination complexes) molecules/ions. Electron pair wave function, V.B. theory and its application to  $H_2$  molecule, comparison of V.B. and M.O. theories

Module-4: Coordination Chemistry-I

Experimental evidence of metal ligand overlap, spin orbit coupling constant and inter electronic coupling parameters in complex ion terms-vs-free ion terms, Nephelauxetic effect, adjusted CFT, hole formalism, interpretation of general features of the electronic absorption spectra, vibronic coupling, intensity, stealing, band broadening, effect of substitution, electronic structure and bonding of octahedral and tetrahedral complexes on the basis of simple symmetry and overlap principles, the MO energy level

diagrams (with appropriate symmetry designation) of these complex, magnetic property: spin and orbital moment, spin orbit coupling, quenching of orbital moment.

**Module-5: Coordination chemistry-II**

Thermodynamics and stoichiometric stability constants of metal ligand complexes. Determination of composition and stability constants of complexes by pH-metric, spectrophotometric and polarographic methods, Irving-Williams order, conditional stability constants and their importance in complexometric (EDTA) titration of metal ions. Statistical and nonstatistical factors influencing stability of complexes in solution, Labile and Inert complexes. Stability and reactivity of mixed ligand complexes, chelate effect, templet effect and macrocyclic effect.

**Module-6: Bioinorganic Chemistry**

Essential elements in Biology (major and trace), beneficial and toxic elements, role of metal ions, bioenergetic principle and role of ATP.  $O_2$ -uptake proteins: hemoglobin, myoglobin, hemerythrin and hemocyanin, structure, function and model study. Electron transfer protein: Fe-S proteins, metal ions transport and storage proteins: ferritin, transferrin, ceruloplasmin, transport across biological membrane-  $Na^+K^+$ -ATPase, ionophores. Hydrolytic enzymes: carbonic anhydrase, carboxypeptidase, urease. Metal dependant diseases: -Wilson's disease, Alzheimer disease. Transition metal complexes as drug.

**Module-7: Organometallic chemistry-I**

Application of 18-electron and 16-electron rules to transition metal organometallic complexes, Ligands in organometallic chemistry; synthesis, bonding and reactivity of metal alkyl, -alkene, -alkyne, -allyl, -carbene, carbene and carbide complexes, Agostic interaction, Stereochemical non-rigidity and fluxional behaviour of organometallic compounds with typical examples

**Module-8: Chemistry of d-block element:**

Chemistry of Ti-Zr-Hf, V-Nb-Ta, Cr-Mo-W, Mn-Tc-Re, Ru-Rh-Pd, Os-Ir-Pt with reference of electronic configuration, oxidation states, coordination number, aqueous chemistry, redox behavior, Iso and heteropolyoxometalates with respect of V, Mo, and W: synthesis, reactions, structures, uses. Dinitrogen and dioxygen complexes: synthesis structure and bonding and reactivity, bonding of  $Re_2Cl_8^{2-}$  (with M.O.). Synthesis, structures bonding and properties of molybdenum blue, Tungsten blue, ruthenium blue, Platinum blue, tungsten bronze, ruthenium red. Creutz-Taube complex, Vaska's complex. Nb, Ta halide clusters. Electronic configuration, oxidation state and comparative study. Stabilization of uncommon oxidation states of transition metals by complex formation- Fe(IV), Ni(III), Ru(IV), Os(IV), Pd(III/IV), Pt(III), Synthesis and structures

Module-9: Chemistry of Main Group Element

Clusters in elemental state, cluster classification, skeletal electron counting. Boron hydride: boranes, structure bonding (M.O. description of  $B_2H_6$  and  $B_2H_6^{2-}$ ) and Lipscomb's topology, 'styx' system of numbering, nomenclature and carborane, metalloboranes, metallo carborane synthesis and structure Wade's rules, borane compounds of potential medicinal interest; boron neutron capture theory (BNCT); Allotropes of Carbon- $C_{60}$  and compound (fullerenes), Intercalation compounds of Graphite Carbon nanotubes, synthesis, properties, structure-single walled, multiwalled, applications graphene

Module-10: Analytical chemistry

Errors in quantitative analysis, types of errors, handling of systematic errors, Random errors: distribution, standard deviation, confidence limits of the mean, presentation of the results, propagation of random error. Solvent extraction: principle, distribution ratio, partition coefficient, successive extraction and separation; effect of pH, use of different organic reagents. Chromatography: general principle, classification, mathematical relations of capacity, distribution constant, retention time; chromatogram, band broadening and column efficiency, column resolution, paper chromatography, thin layer chromatography (TLC), size exclusion chromatography, ion exchange chromatography, capillary electrophoresis

Paper-IV  
Chemical Technology  
F.M.-100

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- Module-1: Fluid Dynamics  
Fundamental principles of fluid mechanics, Newtonian and NonNewtonian fluids. Streamline and turbulent flow, Pressure drop calculation for cflow through pipes and channels, Hagen-Poiseuille equation, Bernouli equation
- Module-2: Filtration & flow measuring instrument:  
Flow measuring instruments, filtration and different filter
- Module-3: Heat Transfer Operation  
Heat Transfer by conduction, steady and unsteady state of heat transfer, heat transfer by convection, Natural and forced convection, Heat transfer by radiation, Heat emission by absorpction by black, natural and grey bodies.
- Module-4: Unit Processes  
Unit processes in organic synthesis including nitration, hydrogenation, oxidation, sulphonation, esterification and polymerization
- Module-5: Stoichiometry:  
Industrial stoichiometry, material and energy balance, solution of problem,chemical reactions, isothermal, adiabatic and nonisothermal and non-adiabatic, Design equation. Heat and Mass transfer effect on catalytic reaction.
- Module-6: Principal of diffusion and mass transfer, mechanism of mass transfer, simultaneous heat and mass transfer, Fick's law application.
- Module-7: Ore Processing /Benefication  
Definition of an ore, types of ores, Operating steps involved in ore processing/dressing/benefication: coominution, sizing and screening concentrstion and filterprocessing. Different process of concentration of ore minerals. Benefication of Pb-Zn-Cu ore, Iron ore, Zn ore etc. Beach sands and graphite, leaching as means of ore processing.
- Module-8: Fuel  
Solid, liquid and gaseous fuels, coal origin, proximate analysis and ultimate analysis, combustion, Petroleum and refineries, products, synthetic liquid fuels, Bergious process, Fisher Tropsch process.
- Module-9: Refractory materials, nomenclature, classification, acidic, basic and neutral refractories, production and important properties and uses

**Syllabus of M.Sc. Part-I, Chemistry (D.D.E)**  
**New-Syllabus (From-session: 2014-15)**

|                   |                  |
|-------------------|------------------|
| <b>Practical:</b> | <b>200 Marks</b> |
| 6. Physical:      | 50               |
| 7. Organic:       | 50               |
| 8. Inorganic:     | 50               |
| 9. Industrial:    | 25               |
| 10. Computer:     | 25               |

**Examination Hour:** 6 hrs (Physical Organic, Inorganic (2 days each), 3 hrs (Industrial), 2 hrs (computer))

## List of Physical Experiments (Part-I)

F.M.-50 (17+18+5+5+5)

1. Determination of Critical Solution Temperature of Phenol water System
2. Determination of Dissociation constant  $pK_a$  and  $pK_1$  and  $pK_2$  of weak monobasic acid and dibasic acid (acetic acid, benzoic acid) ph-metrically
3. Determination of exact concentration of acid mixture (HCl & Oxalic) conductometrically
4. Determination of exact concentration of KCl solution of N/10 order by  $AgNO_3$  potentiometrically and determination of solubility product of AgCl
5. Determination of partition co-efficient of Benzoic acid between water and benzene. Hence show that benzoic acid dimerizes in benzene layer.
6. Determination of E of quinhydrone electrode
7. Study the kinetics of Inversion of cane sugar by polarimeter
8. Verification of Lambert-Beer's Law ( $KMnO_4$  solution or  $K_2Cr_2O_7$  solution)
9. Study the kinetics of iodination of acetone in presence of acid. Hence find out the order with respect to iodine or acetone.
10. Conductometric titration of  $AgNO_3$  and KCl
11. Determination of dissociation constant and  $\lambda_0$  of a weak monobasic acid conductometrically and verification of Ostwald's Dilution Law
12. Conductometric determination of concentration of KCl, HCl and  $NH_4Cl$  in a mixture (By NaOH solution and  $AgNO_3$  solution)
13. Determination of dissociation constants ( $K_1$ ,  $K_2$ ,  $K_3$ ) of  $H_3PO_4$  by ph-meter.
14. Determination of solubility product of  $BaSO_4$  conductometrically.

15. Determination of  $E^0$  value of  $\text{Ag}^+/\text{Ag}$  electrode and activity co-efficient of different aqueous  $\text{AgNO}_3$  solutions potentiometrically.
16. Determination of the order and rate constant of the reaction between  $\text{K}_2\text{S}_2\text{O}_8$  and  $\text{KI}$  and study the influence of the rate constant (Two days)
17. Study the kinetics of alkaline hydrolysis of crystal violet. Determination of the order with respect to  $\text{NaOH}$  and salt effect on the system (Two days)
18. Determination of the rate constant and the order of the reaction of  $\text{KBrO}_3$  and  $\text{KI}$  in acid medium (One and half day)
19. Determination of composition of complexes (Ferri-salicylate complex/Ferrous-orthophenanthroline complex) by Job's method

M.Sc. Part-I, Organic Practical

F.M.-50 (20+10+10+5+5)

- A. Qualitative Analysis of Solid Organic Compounds (At least 6 samples)-
1. Detection of Special elements (N, Cl, Br, I, S): Solubility Test
  2. Systematic Analysis to detect the functional group: alcohol, phenolic OH, -COOH, -COH, -CO, -COOMe/Et, -NO<sub>2</sub>, -NH<sub>2</sub>, -NH<sub>2</sub>Me, N-substituted amino, imido groups, unsaturation (C=C), Ar-hydrocarbons and halogenated derivatives through group classification survey
  3. Preparation of crystalline derivatives to identify the compound
- B. Preparation: Preparation of pure organic compound by single step or two step procedure then submission of crystallized products
- c. Sessional worke
- D. Laboratory Note Book
- E. Viva(To be jointly conducted by the external and internal examiners during the examination)

