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

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

A. Theory: **400 Marks**

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)

(Core Faculty) (H.O.D) (DIRECTOR)

Chemistry

Distribution of Marks for written Examination Paper Wise (Both for Part – I & II):

Sl. No.	Theory : 100 Marks	Question Marks
1	Answer any 08 Questions out of 16 Questions Carrying 02 marks of each	8 x 2=16
2	Answer any 08 Questions out of 12 Questions Carrying 04 marks of each	4 x 8 =32
3	Answer any 04 Questions out of 08 Questions Carrying 08 marks of each	4 x 8 = 32
4	Internal Assessment	20
Total		100 Marks

Syllabus at a glance

Part I: 600 marks 48 credits		Part II : : 600 marks 48 credits		Total : 1200 marks 96 credits	
Theory	Practical	Theory	Practical	Theory	Practical
400	200	400	200	800	400

M. Sc. Part I

TYPE	PAPER	TOPIC	Credit	FULL MARKS
Theoretical	I	Physical	8	100
	II	Organic	8	100
	III	Inorganic	8	100
	IV	Industrial	8	100
Practical	I	Physical	4	50
	II	Organic	4	50
	III	Inorganic	4	50
	IV	Industrial & Computer	4 (2+2)	50

M. Sc. Part II

SPECIALIZATION	TYPE	PAPER	TOPIC	Credit	FULL MARKS
Organic	Theory	V	Organic	8	100
		VI	Organic	8	100
		VII	Organic	8	100
		VIII	Polymer Science	8	100
	Practical	-	Organic practical	8	100
	Project		suggested by	8	100

		-	appropriate project guide		
Physical	Theory	V	Organic	8	100
		VI	Organic	8	100
		VII	Organic	8	100
		VIII	Polymer Science		100
	Practical	-	Physical	8	100
	Project	-	suggested by appropriate project guide	8	100

Paper-1

Physical Chemistry

F.M.-100

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 theorm, 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, Homogeneouis and heterogeneious catalysis, enzym catalysis and inhabition, auto catalysis, ascillatory 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 Spectrscopy-1:

General Introduction, Nature of Electro amgnatic 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, Anhermonic oscillator model, Rotational Vibrational spectra of diatomic molecules.

Module-10: Molecular Spectroscopy-2:

Raman Spectroscopy: Introduction, Classical thepry of Raman scattreing, 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 Spectroscppy: Moand LCAO (Term Symbol (Linear Molecules) of Molecular States, Electronic energy state of polyatomic molecules, Radiative and Nonradiative precess, Franck-Condon principle.

Paper-II

Organic Chemistry

F.M.-100

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, Wood Word Hofmann 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 butadine 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 interections 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 systhesis of tritepenes: biogenetic isoprene rule: monocyclic, bicyclic, tricyclic and pentacyclic ring systems, Fragmentation reaction, Remote functionalization:biomimetic reactions/template effect, examples fuctional groups interconversion, Multicomponent reactions: Definition, early examples, Passerine reaction, Ugi reaction, Olefinmetathesis 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, Sharpness asymmetric epoxidation, AD-mix, Tranaformation of expoxides, Organophosphorus reagents, organo sulfer 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 systhesis.

Module-5: Natural Products-Terpenoids:

Terpenoids: Isoprene rules, acyclic monoterpenoids, central geraniol neral, linalool monocyclic monoterpenoids: terpeinol, structure elucidation, synthesis and biogenesis. Higher terpenoids:P sesquidi-, ssester-, 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, hrlicity, 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

Modsule-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 rearrangementrs 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}H NMR, UV, IR) in structure determinastion of organic compounds, Aromaticity, Anti aromaticity, Homoaromaticity, Annulene systems

Paper-III

Inorganic Chemistry

F.M.-100

Module-1: Symmetry and Group theory-I

Groups and their properties-the concept of groups; subgroups classes and their related theorems; commutative (abellian) 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 dipolemoment 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-π^* and π-π^*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 Vab 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 comploxometric (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 (malor and trace), beneficial and toxic elements, role of metal ions, bioenergetic principle and role of ATP. O_2-uptake proteins: hemoblobin, myoblobin, hemerythrin and hemocyanin, structure, function and model study. Electron transfer protein: Fe-S proteins, metal ions transport and storage proteins: ferritin, transferin, ceruloplssmin, transport across biological membrane- Na^+-K^+-ATP Pase, ionophores. Hydrolytic enzymes: carbonic anhydrase, carboxypeptidase, urease. Metal dependant diseases:-Wilson's disease, Alzheimer disease. Transition mrtal complexes as drug.

Module-7: Organometallic chemistry-I

Application of 18-electron and 16-electron rules to transition metal organomatallic complexs, Ligands in organometallic chemistry; synthesis, bonding and reactivity of metal alkyl, -alkene, -alkyne,-allyl,-carbene, carbine and carbide complexes, Agostic interaction, Stereochemical non-rigidty and fluxional brhaviour 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 halideclusters. Electronic configuration, oxidation state and comperative study. Stabilization of uncommonoxadation 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 systhesis and structure Wade's rules, borone compounds of potential meditional interest; boron neutron capture theory(BNCT); Allotrops of Carbon-C_{60} and compound (fullerenes), Intercalation compounds of Graphite Carbon nanotubes, synthesis , properties, structure-si9ngle walled, multiwalled, applications graphene

Module-10: Analytical chemistry

Errors in quantitative analysis, types of errors, handelling of systematic errors, Random errors: distribution, standard deviation, confidential limits of the mean, presentation of the results, propagation of random error. Solvent extraction: principal, 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

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 absorption 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 Practical(D.D.E)

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

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 exact concentration of KCl solution of N/10 order by $AgNO_3$ Potentiometrically and determination of solubility product of AgCl.

3. Verification of Lambart-Beer's Law ($KMnO_4$ solution or$K_2Cr_2O_7$ solution).
4. Determination of dissociation constant and λ_0 of a weak monobasic acid conductometrically and verification of Ostwald's Dillution Law.

5. Conductometric determination of concentration of KCl, HCl and NH_4Cl in a mixture(By NaOH solution and $AgNO_3$ solution)

6. Determination of dissociation constants (K1, K2, K3) of H_3PO_4 by ph-meter.
7. Determination of solubility product of $BaSO_4$ conductometrically.

8. Determination of E^0value of Ag^+/Ag electrode and activity co-efficient of different aquous $AgNO_3$ solutions potentiometrically.
9. Determination of the rate constant and the order of the reaction of $KBrO_3$ and KI in acid medium(One and half day).
10. Determination of Dissociation constant pka and pk1 and pk2 of weak monobasic acid and dibasic acid (acetic acid, Oxalic acid) ph-metrically.

11. Determination of exact concentration of acid mixture (HCl & Oxalic) conductometrically.

12. Determination of partition co-efficient of Benzoic acid between water and benzene. Hence show that benzoic acid dimerizes in benzene layer.

13. Determination of E of quinhydrone electrode.

14. Study the kinetics of Inversion of cane sugar by polarimeter.

15. Study the kinetics of iodination of acetone in presence of acid. Hence find out the order with respect to iodine or acetone.

16. Conductometric titration of $AgNO_3$ and KCl.
17. Determination of the order and rate constant of the reaction between $K_2S_2O_8$ and KI and study the influence of the rate constant(Two days)

18. Study the kinetics of alkaline hydrolysis of crystal violet. Determination of the order with respect to NaOH and salt effect on the system(Two days)

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, $-NO_2$, $-NH_2$, $-NH_2Me$, N-substtituted 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)

M.Sc. Part-I, Inorganic Practical

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

(Two days examination- 6 hours per day)

A. Qualitative Analysis: Detection of six radicals from a mixture one from less common ion

(Except-Ag(I), Hg(I), Pb(II), As(III), AS(IV), Sb(IV), Less common ion- V(III), V(V),Zr(IV), Mo(VI), W(VI), Ti(IV), Th(IV)) 20

B. Quantitative analysis: 20

i) Estimation of Cu(ii) and Zn(ii) in brass by volumetry and gravimetry method
ii) Estimation of manganese in pyrolusite
iii) Gravimetric estimation of Ni(ii) as DMG complex
iv) Volumetric estimation of Mn(II)/Fe(III)

C. Viva Voce 05

D. Laboratory Note Book 05

M.Sc. Part-I,Industrial Chemistry Practical

F.M.: 25

1. Study and Use of orifice meter, venture meter, point tube Rayleigh 15
    1. Distillation and other skills. Bombcalorimeter, Junckers calorimeter
    2. Determination of surface area by air permeability method
    3. Determination of viscosity of liquid by falling sphere method
    4. Determination of viscosity of fuel oil(Red woods viscometer)
    5. Proximate analysis of coal samples
    6. Orsat analysis
    7. Determination of flash point of a fuel oil
    8. Determination of diffusion coefficient of liquid vapour through air by Stefens Method
    9. Distillation of binary liquid mixture to verify Reileigh equation
2. Laboratory Note Book 05
3. Viva Voce 05

M.Sc. Part-I,Computer Practical

Full Marks: 25

Theoy Based Practical

History of development of computer mainframes, minis, micros, and Supercomputer. Computer Hardware, CPU and other peripheraldevices(Input/output and auxiliary storage devices), introduction to software and programming languages, Details of Fortran77-and its application in solving simple problems like solution of quadratic equation, summationnhotwral numbers, finding Harvard deviation, strong of numbers, 1^{st} order reaction, software packages: d BASE LOTUS, WORD STAR, WINDOW

Question Pattern: Short question multiple choice

Part-II
Organic Special
Paper-v

SLM 1. **Stereochemistry-Unit-1:**

Conformations and chemical reactivity-Curtin-Hammett principal, its derivation under different conditions and applications, quantitative treatment of mobile system, Winstein Holress equation and Eliel equation-their applications; strain and Strain , allylic 1,2-and 1,3-strain (in pseudo allylicsyatem also), their applications

SLM 2. **Stereochemistry-Unit-2:**

Fused ring system, trans and cis declaims, conformation , steroid and non steroid conformation, symmetry, torsion angale enthalphy , entropy, free energy, substituted declaims q-methyldeclains and 9,10 dimethyldececalins, decalones; conformation of cis-octalins trans-octalins.

SLM 3. **Stereochemistry-Unit-3:**

Stereochemistry of 4-10 membered rings, transanular reactions; perhydrophenanthrenes and perhydroanthracenes conformations, energy, summetry and optical activity, relative stability,stereochemistry of perhydrodiphenic acids and perhydrophenanthrenes, conformations of some triterpenes.

SLM 4. **Stereochemistry-Unit-4:**

Modern concepts of nucleophilic addition to carbonyl compounds, felkin model(torsional strain) Burzi Dunnitz trajectory,cieplaak model,examples.

SLM 5. **Stereochemistry-Unit-5:**

Optical rotation,specific and molecular rotations-their units, Brewster rule, Lowe's rule , origin of optical rotation, circular birefringence, optical rotator dispersion (ORD) octant rule, axial haloketone rule-application(octant projection diagram); circular dichrosm(CD) differerntial diachronic absorption, specific ellipcity and molar ellipticity , application of CD—helicity rule ,exciton chirality (dibenzoate chirality rile)Davydor splitting-applications with different steroidal glycols.

SLM 6. **Pericyclic reaction:**

Pericyclic reactions and applications of MO theory to organic chemisrtry: Electrocyclic reactions, sigmatropic rearrangement, cycloaddition and cycloreversion reaction, cheletropic reactions, ene reaction .

Frontier Molecular Orbital theory, concept of aromaticity of transition states, orbital correlation diagram, Huckel MO theory-MO's of chain and rings alternants and nonalternants.

SLM 7. Linear Free Energy Relationship-Unit-1:

Linear Free Energy Relationship: Quantitative correlations of rate and equilibria. Linear Free Energy Relationships with special reference to Hammett,Taft, Yukawa-Tauno and Gruwald-weinsrein equations.

SLM 8. Linear Free Energy Relationship-Unit-2:

Application of Linear Free Energy Relationship to aromatic, aliphatic,polynuclear and hetero-aromatic systems. Multiparameter correlations(elementary ideas).Electrophilic substitution in aliphatic systems(SE1 and SE2 reactions).

SLM 9. Organometallic chemistry:

Preparation and reactions of pi-complexes,heptonumbers, rules for nucleophilic addition to complexes, application to typical synthesis. Use of transition metal: organometallics in organic synthesis.

SLM 10. Organic Synthesis:

Organic synthesis strategy, retrosynthetic analysis: the disconnection approach.

Part-II
Organic Special
Paper-VI

SLM 1. Organic photochemistry-Unit-1:

Organic photochemistry: Fundamental concepts, jablonski diagram, photochemistry of organic compounds, Norrish type-I and Norrish type-II processes, patterno Buchi reaction, Barton reaction, addition reaction, oxidation reaction.

SLM 2. Organic photochemistry-Unit-2:

Photochemical reduction, substitution reaction, cis-trans isomerism, photochemistry of butadiene, di-pi methane rearrangement and related processes.

SLM 3. Bioorganic and supramolecular chemistry-Unit-1:

Crown ethers: discovery, nomenclature, synthesis, properties and application. Cryptands: structures and applications. Molecular recognition: definition, examples of molecular recognition utilizing H-bonding, electrostatic, solvophobic, pi-pi interaction,etc.,application of molecular recognition.H-bonding in molecular organization, chiral recognition, introduction to molecular mechanics calculation and its use in the design of molecular receptors.

SLM 4. Bioorganic and supramolecular chemistry-Unit-2:

Cyclodextrins: structure, property, application. Enzymes: enzyme kinetics, mechanism; application of enzymes in organic synthesis, model enzymes based on cyclodextrins.

SLM 5. Bioorganic and supramolecular chemistry-Unit-3:

Self-assembling system: micelles, reverse micelles; vesicles,fiber's and tubules; amphiphiles, bola-amphiphiles,self replication.

Gels: definition, classification, examples, study of the morphology and rheology of gels , applications.

Chemical sensors: photo-responsive system, Dye sensitized solar cell, liquid Crystals, Molecular electronic device, organic conductors.

SLM 6. Biological Active Molecules:

Antibiotics , penicillin, cephalosporin, streptomycin, structure, synthesis and biological active to bacteria.

SLM 7. Peptides and Nucleic acids:

Peptides and proteins: structure and functions; α-helix, β-pleated sheet, β-turn,3.10 helix, Ramachandran plot.

Nucleic Acids: Structure and functions; replication of nucleic acids.

SLM 8. Vitamins and Co-enzymes:

Vitamins A1, B1, C, K, coenzymes, NAD,FAD and reactivity of different vitamin in biological reactions.Chemistry of nucleosides, nucleotides and ATP, elementary structure and various types of RNA's in protein biosynthesis.

SLM 9. Green Chemistry:

The current status of chemistry and the environment. What is green chemistry? How green renewable are related to sustainability.Principles,methodologies and techniques in green chemistrty. Synthesis in aqueous media, catalytic methods in synthesis,Examples of green chemistry. Future trends in green chemistry.Unconentional energy sources in synthesis: solar energy.

SLM 10. Heterocycles-2:

Heterocycles: Synthesis and reaction: Generalized approach to the synthesis of heterocycles possessing 5-,6- and 7-membered rings with one or two heteroatoms per ring.Reactions of heterocycles: oxidation and reduction reaction with electrophiles,nucleophiles and other reactive intermediates with typical monocyclic and fused ring systems as examples.

Part-II
Organic Special
Paper-VII

SLM 1.

Detailed study of ^{1}H NMR and preliminary aspect of ^{13}C NMR, CW and FT techniques.

SLM 2.

NMR spectroscopy: principles, Relaxation phenomenon, factors influencing chemical shift and coupling constant, simplification of complex spectrum, NOE, Rotating frame of reference.

SLM 3.

Mass-spectroscopy combined application of spectroscopical methods to organic molecules: principles of Mass spectroscopy, Different techniques, fragmentation modes.

SLM 4.

Combined application of spectroscopic technique (UV, IR, NMR, MS) in elucidation of structure and study of reaction of organic compounds.

SLM 5. Alkaloids:

Indole alkaloids-biogenesis and chemistry of representative members such as yohimbine, reserpine, strychnine, other alkaloids : quinine, morphine, and its derivatives.

SLM 6.

Acetogenesis, prostaglandins and porphyrins: structure, reaction, synthesis, and biosynthesis of typical prostaglandins.

SLM 7. Flavanoids:

Biogenesis and chemistry of acetogenesis-coumarins, Flavanoids, lignin and porphyrin, some typical examples.

SLM 8. Biogenesis of terpinoids and steroids:

Structure elucidation and synthesis of some representative members mono, di- and tri-terpenoids from the following: Logamin, santonin, Germacrane, Zerumbone, farnesol, gibberalline, abietic acid.

SLM 9.

Squalene, presqualene, amyrins and lupeols. The use of these terpenoids as renewable nanbuilding block for nano-materials and nano-devices. Steroids: Nomenclature, representative members such as Cholesterol, sex hormones and artificial hormones.

Part-II
(Organic Special/physical special)
Paper-VIII

SLM 1. High polymer system:

Basic principles, definition, origin and classification of polymers, structure-property Relationship,Rubber, plastic and fibres.

SLM 2. Importants of some fundamental quantites:

Polymer characterization: End groups, head to tail structure.Molecular weight and molecular weight distribution. Number average, weight average and viscosity average molecular weight of polymers; polydispersity index.

SLM 3. Step growth and condensation polymerization:

Functionality principles,kinetics and mechanism of step growth polymerization. Molecular weight control in linear stepwise polymerization.Molecular weight distribution in condensation polymers.Carothers equation and flory equation,prediction of gel point.

SLM 4. Chain Growth or additional polymerization:

Free radical and ionic(cationic and anionic) poloymerization and their kinetics and mechanism; degree of polymerization and its control,chain transfer.

SLM 5. Additional aspects of polymerisation:

Copolymerzation, stero regular polymerization. Techniques of polymerization. Mass, solution suspension, and emulsion polymerization.

SLM 6. Plastic Technology:

Materials; Synthesis, properties, uses and application of polyethylene, polypropylene, ethylene copolymers, polystyrene,polyvinyl chloride, acrylics, acetal resins, cellutosics, polycarbonates.

SLM 7. Resins:

Phenol-formaldehyde resins, alkyd resins, linear and fibre forming polyester,nylon polyamides, epoxy resina.

SLM 8. Processing technology:

Polymer additive,mixing and compounding.

SLM 9. Rubber Technology:

Materials, natural rubbers, styrene-butadiene rubber(SBR) , polychloroprene, polybutadiene, nitrile rubber, ethylene propylene rubber, EPDM rubber.

SLM 10. Substituted polymer and rubber:

Chlorosulfonated polyethylene (Hypalon), polysulphide rubber, butyl rubber. Silicone resins and rubber: synthesis, properties, uses and application.

Part-II

PRACTICAL

(Organic Special)

New syllabus(session 2014-15)

Full Marks: 100, two days (6 hours per day)

Unit-01:

Separation followed by systematic qualitative analysis of two component mixture or two solids.Pure samples of the compound and their suitable crystalline derivatives are to be submitted along with proof of their purity (by TLC or paper chromatographic analysis). At least 5 mixture to be analysed.

[30]

Unit-02:

Qualitative Analysis of an organic liquid substance leading to its identification.

[20]

Unit-03:

Preparation of organic compounds by typical multistep procedure (at least four synthetic sequences to be performed). Samples of final products and intermediates to be submitted. UV, and IR spectra of products to be recorded and interpreted.

[30]

Unit-04: Sessional

To be awarded by the class teacher on the basis of performance during course work.

[10]

Unit-05: Viva-Voce (during examination)

To be conducted jointly by the internal and external examiners.

[10]

M.Sc Part-II

PROJECT WORK

(Organic Special)

New syllabus(session 2014-15)

Full Marks: 100, 30-40 days (3 hours per day)

Unit-01: Topics of investigation to be assigned by instructor/class teacher

Duration of work will 30-40 days(3 hours per day).Students have to submit the report of his/her work in the form of a thesis(in duplicate).These will be adjudicated jointly by a board of examiners consisting of the one internal and one external examiners.

[60]

Unit-02: Vica-Voce

To be conducted jointly by the internal and external examiners on the thesis submitted under **01**.

[20]

Unit-03: Seminar

Every student has to deliver a seminar lecture (20-30mins duration) in the department on topics assigned by the class teacher or on any topics in chemistry of contemporary interest. Evaluation will be done by the class teacher based on individuals performance in the seminar.

[20]

Part-II
PHYSICAL SPECIAL
Paper – V

Module – 1: Electrical and Magnetic properties

Limitations of Debye equation, Curie-Weiss point and ferroelectricity; Onsager's theory of internal field. Kirkwood's equation and structure of water, dielectric dispersion and loss. Dielectric effect on emission and absorption spectra. Lippert-Mataga equation, frequency dependent dielectric property. Debye semi-circle, relaxation time, deviations from Debye's theory, time resolved spectroscopic studies and dielectric relaxation effect.
Quantum mechanical theories of dia and para-magnetism anisotropy, ferro- and antiferro-magnetism.

Module – 2 : Quantum mechanics-I

Matrices related to advanced quantum mechanics matrix representation of operators, projection operators, electron spin, antisymmty principle, matrix eigenvalue problems, spin operators and their matrix representation. Matrix representation of schrodinger equation.

Module – 3 : Quantum mechanics-II

Quantum mechanics of many electron atom excluding spin, Helinm atom, N-electron atom, Independent particle model, Hartree Self consistant Field (SCF) method derivation of total electronic energy expression in terms of hartree orbital energy, validity of Koop man's theorem, Slater type orbital, elementary "Idea of Gaussian orbitals"

Module –4 : Quantum mechanics-III

Quantum mechanics of many electron atom including spin, derivation of total electronic energy of a system containing 2N electrons, Hartrce-Fock Theory, Unitary Transformations, Validity of Koopman's theorem, Roothaan-Hartrce-Fock theory and its applications, derivation of total electronic energy in terms of Hartree-Fock orbital energy.

Module –5 : Quantum mechanics-IV

Approximate methods in quantum mechanics, Variational principle, Eckares Rule**.**Linear variational theorem, Huckel Theory applications, analytical methods for linear and Eckarts Rule, Cyclic polyenes, Huckel theory of systems containing hetero atoms. Extended Huckel theory and its applications.

Module –6: Quantum mechanics-V
Parturbation Theory, derivation of perturbation equations, first order non-degenerate and degenerate perturbation theory, applications, enharmonic oscillator, non rigid rotator, Hydrogen molecule ion , Stark effect.

Module –7 : Group Theory

Group Theory symmetry properties, symmetry transformations, symmetry groups sub groups, finite and continuous groups, Matrix representation of point group and transnational groups, Reducible and verifiable representations, characters, projection operation, direct produced representation, Orthogonatits theorem, character level, applications of G.T. to symmetry, spectator.

Module –8 : Solid 1

Free electron theory of metals (classical theory and quantum theory); Electrical conductivity of metals, X-Ray diffraction necessary condition, Laue's diffraction, atomic scattering factor and geometrical structure factor, Lattice vibration, phonons and excitons, Hall effect. (briefly)

Module –9 : Solid 2

Band str of metals, conductors, semiconductors (n-type, p-type and n-p function), superconductors and insulators, Lattice defects (mainly Schotthy defect and Frenkel defect), Color Centre : F-Centre, V-Centre, $F^{/}$-centre etc.

Part-II
PHYSICAL SPECIAL
Paper – VI

Module – 1: Statistical Mechanics-I

Concept of ensemble and phase space, ergodic hypothesis; microcanonical ensemble : partition function, temp^{r}: canonical ensemble: distribution, probability and partition function, partition function and different thermodynamic state functions Gibbs paradox. Molecular partition fn: translational, rotational, vibrational, electronic and nuclear.

Module –2: Statistical Mechanics-II

Principle of equipartition of energy, chemical eqm system of interacting particles, imperfect gas. Grand canonical ensemble : Nature of quantum particles, Bose Einstein and Fermi-Dirac statistics; specific heat of electron gas. Bose-Einstein condensation. Quantum statistics, density matrix.

Module-3: Non-equilibrium thermodynamics

Entropy production in irreversible processes, Onsager reciprocal relations, principle of microscopic reversibility, thermonuclear pressure difference and thermonuclear effect, cyclic and oscillatory reactions, non-linear region, higher order symmetries.

Module –4: Mossbauer spectroscopy

Mossbauer spectroscopy principle, experimental set up, center shift, quadrupole interaction, magnetic interaction, Mossbauer spectra of iron compounds, Applications study of spin, oxidation states, bonding and spin transitions.

Module –5 : Advanced Electrochemistry

Modifications and extensions of the Debye-Huckel theory, surface tension of electrolytic solutions, theories of solvent interaction, non-stationary processes in electrolytic solutions, hydrogen overvoltage, thermodynamics of ideally polarized electrodes, metal electrolyte and semiconductor electrolyte interfaces, Fuel cells

Module –6 Advanced chemical kinetics-I

Transition state theory, thermodynamic formulation of reaction rates, potential energy surface and contour reaction path; valley and saddle point – activation energy; Quantitative treatment of TST by using partition function; statistical formulation of chemical kinetics, equilibrium formulation, derivation of expression for specific reaction rate, entropy of activation.

Module –7: Advanced chemical kinetics-II

Reactions in molecular beams; Reactions and shock waves. Application of absolute reaction rate theory in viscosity. Reactions between ions influence of solvent dielectric constant, (double sphere model) pre—exponential factors, single sphere activated complex, influence of ionic strength. Diffusion controlled reactions (full microscopic diffusion control and partial microscopic diffusion control)

Module –8 : Macromolecules

Molecular weight of polymers, molecular weight determination by light scattening, viscosity, osmometry, sedimentation and diffusion measurements. Thermodynamics of polymer solution (Flory-Huggins Theory). Kinetics of polymerization.

Module –9 : Biopolymers

Structure of biomoleculs : 1) Proteins-building blocks, peptide bonds, primary, secondary, tertiary, quaternary structures, Phi-Psi map. 2) Nucleic acids – A,B,Z Conformations, t-RNA conformation, Carbohydrates and lipids biomembranes. Methods for determination of molecular weight of biopolymers a) SDS-PAGE (for proteins), b) agarose gel method (for nucleic acids). Techniques to study biomolecules CD, ORD, fluorescence, IR and Ramen spectroscopy (simple applications)

Part-II
PHYSICAL SPECIAL
Paper – VII

Module – 1: Rotational spectra of Polyatomics

Rotational spectra of polyatomics : Spherical top, symmetric top, and asymmetric top molecules. Internal retation, nuclear spin and rotational energy levels. Stark effect, Coriolis coupling.

Module –2: Vibration of polyatomic molecules

Vibration of polyatomic molecules: Normal modes and their symmetry, overtones, combination bands and hot bands. Introduction to normal co-ordinate analysis, localized group vibrations non-genuine vibrations. Torsional oscillations. Fermi resonance.

Module –3: Electronic Spectroscopy

Electronic spectroscopy : Energy levels, orbital and spin selection rules, vibronic transitions, polarizations. Vibrational progressions, Franck Condon principle (quantum mechanical formulation), geometry of the excited states.
Polarisation of Raman lines, mutual exclusion principle and its application to molecular structure determination. Resonance Raman, Hyper-Raman, and stimulated Raman effect.

Module –4: NMR Spectroscopy

Nuclear energy levels in a magnetic field, nuclear magnetic resonance (NMR) and its instrumentation; Bloch equations and their solutions; chemical shift and nuclear shielding (diamagnetic and paramagnetic), fine structure and spin-spin interaction, shape of spectral lines, spin lattice relaxation time and line width. Echo experiments, NMR of solids, NMR imaging, Elementary idea of CIDNP.

Module-5: EPR spectroscopy

Energy levels of a spinning electron in a magnetic field, principle of EPR spectroscopy and instrumentation, X-band and Q-band spectra, linewidth, hyperfine splitting, g-anisotropy and hyperfine splitting, EPR of triplet states, EPR spectra of paramagnetic salts and organic radicals (some typical examples), spin orbit interaction and symmetry of crystal field, EPR and delocalization of spin Elementary idea of CIDEP.

Module – 6: Laser and its Application:

General features and properties ; method of obtaining population inversion, Laser cavity modes, Q-switching, mode-locking, example of laser:Rudy laser, Nd-YAG laser, diode laser, He-Ne laser, N_2 laser, Ar –laser, excimer and exciplex lase, Dye laser

Application of laser in Raman spectroscopy: Resonance Raman Effect, Stimulated Raman effect, inverse Raman effect, Hyper Raman effect, Coherent anti stokes Raman effect, Coherent stokes Raman effect, NLO Properties.

Module –7: Photochemistry; Law and its application

Sequence of processes in a photochemical reaction, deactivation of the excited state through different processes; fluorescence phosphorescence, delayed fluorescence, resonance fluorescence, flurescence quenching, determination of radiative lifetime of the excited state-principle and instrumentation, ground and excited state complexation. Franck-Condon principle and mirror symmetry.

Module – 8: Principle of FT NMR spectroscopy

FT NMR Spectroscopy: Fourier transformations (general idea), time domain versus frequency domain, introduction to FT NMR spectroscopy, origin of chemical shift, factors which influence chemical shift, spin-spin splitting, 2D methods, application to structure analysis (simple cases)

Module – 9: Reaction dynamics

Reaction Dynamics : General introduction, molecular dynamics intermolecular collision and its consequence: role of intermolecular potential, collision cross section, reaction cross section energy threshold, reaction probability. Angular distribution in reactive collisions. Scattering in velocity space, electronic energy transfer. Experimental methods- crossed molecular beams Photo-fragmentation spectroscopy, femtochemistry.

Part-II
PRACTICAL
(Physical Special)
New syllabus(session 2014-15)
Full Marks: 100, Two days (6 hours per day)

Unit-01: Physical Chemistry Experiments[Two days(six hours each day) examination]

Total Marks: 70(seventy)

A student has to perform (1) Two experiments each of one day duration, or (2) One experiment is of two day duration.

List of Physical Experiments

1. Determination of standard Potential of $Fe(CN)_6^{3-}$ /$Fe(CN)_6^{4-}$ Electrode.
2. Potetiometric titration of halide (Cl^-, Br^-, I^-) Mixture.
3. Verification of the Onsagar Equation and Determination of Λ_0 (Eqv. Cnductance at infinite dilution) of electrolytes KCl, K_2SO_4, $BaCl_2$).
4. Determination of indicator constant of Bromo Cresol Green by Spectro Photometrically.
5. Study of alkaline hydrolysis of Crystal Violet Colorimetrically. (TWO DAYS)
6. Determination of the rate constant of the decomposition of H_2O_2 at three different temperature and determination of its activation energy of its reaction. (TWO DAYS)
7. Determination of Concentration of two Dyes in a mixture Spectrophotometrically.
8. Conductometric determination of KCL, HCL, and NH_4CL in a mixture. (by NaOH solution and $AgNO_3$ solution)

Unit-02: Sessional [05]
Unit-03: Laboratory Note Book(during examination) [05]
Unit-04: Viva-Voce [20]

M.Sc Part-II
PROJECT WORK
(Physical Special)
New syllabus(session 2014-15)
Full Marks: 100, 30-40 days (3 hours per day)

Unit-01: Topics of investigation to be assigned by instructor/class teacher

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Unit-02: Viva-Voce

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Unit-03: Seminar

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[20]