UNIT-I: QUANTUM CHEMISTRY: (15 Periods)

Discussion of solutions of Schrodinger equation to some model systems e.g. the one dimensional harmonic oscillator, two particle rigid rotator.

Ordinary angular momentum, generalized angular momentum, eigen functions of angular momentum, eigen values of angular momentum, different types of Operators and their uses, addition of angular momentum, spin, antisymmetry & Pauli exclusion principle using Ladder operators. Russel-Saunders terms and coupling scheme, Slater-Condon parameters, term separation energies of the $p^n$ and $d^n$ configuration, magnetic effect: spin orbit coupling and Zeeman effect (splitting).

UNIT-II: SYMMETRY AND GROUP THEORY IN CHEMISTRY AND ITS APPLICATIONS: (15 Periods)

Representation of groups:
• Preparation of matrices and vectors.
• Matrix notations for geometrical transformations.
• Orthogonality theorem and its consequences.
• Reducible and irreducible representations and their relation.
• Preparation of character table for $C_{2v}$ and $C_{3v}$ point groups.

Application of group theory to -
• Transformation properties of atomic crystals.
• Hybridization scheme for $\sigma$ and $\pi$-bonding.

UNIT-III: INORGANIC REACTION MECHANISM (15 Periods)

Introduction:
Labile and inert complexes, factors responsible for lability and inertness of complexes.

Experimental Techniques:
(i) Direct chemical analysis, (ii) Photometry, (iii) Electrometry, (iv) Polarimetry, (v) Isotropic tracer, and (vi) Fast reaction techniques.

Reaction Mechanism of Transition Metal Complex:
Reactivity of metal complexes, ligand replacement reaction: classification of mechanism and energy profile of reaction. Inert and labile complexes, interpretation of liability and inertness of transition metal complexes on the basis of VBT and CFT. Factors affecting the liability of a complex, transition state or activated complex, substrate, attacking reagents electrophilic and nucleophilic, Nature of central atom. Kinetic application of CFT.

Kinetics of octahedral substitution, acid hydrolysis, factor affecting acid hydrolysis, base hydrolysis, conjugate base mechanism, direct and indirect evidences in favor of conjugate mechanism, reaction without metal ligand bond cleavage, and reaction of coordinated ligands.
SEMESTER-II

UNIT-I: MAGNETIC PROPERTIES AND ELECTRONIC SPECTRA OF TRANSITION METAL COMPLEXES: (15 Periods)

Introduction:
Definitions of magnetic properties, types of magnetic bodies, the source of paramagnetism, diamagnetism and Pascal's constant.

The Elementary theory of magnetochemistry: properties of paramagnetic bodies.

Determination of magnetic susceptibility:
(a) Gouy method, (b) Faraday method and (c) Null deflection method.

Magnetic moment:
(I) intrinsic orbital contribution, (ii) Spin orbit coupling, and (iii) Temperature independent paramagnetism (T.I.P.).

UNIT-II : METAL π-COMPLEXES: (15 Periods)
Structure and Bonding, vibrational spectra of metal carbonyls for bonding and structure elucidation, important reaction of metal carbonyls, nitrosylating agents for synthesis of metal nitrosyls, vibrational spectra and X-ray diffraction studies of transition metal nitrosyls for bonding and structure elucidation, important reaction of transition metal nitrosyls, structure and bonding.

UNIT-III : INORGANIC POLYMERS: (15 Periods)
Introduction:
- Definition of polymers and their depiction.
- Types of characteristic of inorganic polymers.

Characterization of inorganic polymers (Physical properties):
- By molecular weights
- Number average
- Weight average
- Molecular weight distribution

Structural features of polymers:
- backbone bonding
- branching and cross-linking
- chemical and stereochemical variability

Crystallinity:
- Importance and requirements, Methods for determining percent crystallinity by Dilatometry, crystallography and X-ray diffraction.

Classification, types of inorganic polymers, synthesis, properties, structures and uses in following polymers:
(i) Polyphosphazenes
(ii) Polysiloxanes
Reference Books:

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M. Sc.-I (CHEMISTRY)
TO COME IN FORCE FROM JUNE-2010
PAPER-II (ORGANIC CHEMISTRY)

Max. Marks: 60 (External – 42 + Internal – 18)   Total Periods: 45

SEMESTER-I

UNIT-I: REACTION MECHANISM & REACTIVE INTERMEDIATES (15 Periods)

Detailed study of organic reaction intermediates. Generation, structure, stability and reactions of –

**Carbocations (Classical and non-classical):**

Phenonium ion, norbornyl system, common carbocation rearrangements. Application of NMR spectroscopy in detection of carbocations.

**Carbanions:**

Mechanism of condensation involving enolates - Aldol, Claisen, Mannich, Benzoin, Perkin, Dieckmann, Michael, Shapiro and Stobbe reactions.

**Carbenes:**

Mechanism of Arndt-Eistert reaction, Wolff rearrangement, Reimer-Tiemann reaction and Bamford Steven's rearrangement reaction.

**Free Radicals:**

Allylic halogenation (NBS), oxidation of aldehydes to carboxylic acids, auto-oxidation, coupling of alkenes and arylation of aromatic compounds by diazonium salts. Sandmeyer reactions. Free radical rearrangements, Hunsdiecker reaction.

UNIT-II: PERICYCLIC REACTIONS (15 Periods)

**Introduction** - Definition, Characterization and Classification of Pericyclic reactions Molecular orbital symmetry, conservation orbitals of ethylene, 1,3- butadiene, 1,3,5- hexatriene and allyl system. Application of symmetry properties, correlation diagram and derivation of selection rules for Electrocyclic reactions- Conrotatory and disrotatory motions, FMO and PMO approach 4n, 4n+2 and allyl systems.

**Cyclo addition Reactions:** Antarafacial and suprafacial additions. 4n and 4n+2 Systems FMO and PMO approach. 2 + 2 addition of ketenes, 1, 3- dipolar cydoadditions.

**Sigmatropic rearrangements:** Suprafacial and antarafacial shifts involving H & C moieties. 3, 3 – and 5, 5- Sigmatropic rearrangements.

UNIT-III: STEREOCHEMISTRY AND CONFORMATIONAL ANALYSIS (15 Periods)

**Concept of isomerism:** Dynamic stereochemistry, prochiral relationships, Resolution of racemic modifications, Stereospecific and stereoselective synthesis, Optical activity in the absence of chiral carbon (biphenyls, allenes and spiranes), Chirality due to helical shape.

**Conformational analysis of cyclohexanes:** Axial and equatorial bond, conformation of monosubstituted cyclohexane derivatives, decalins, perhydro-phenanthrenes, Effect of conformation on reactivity, stereochemistry of the compounds containing N and S.
SEMESTER-II

UNIT-I: ORGANIC REACTIONS (15 Periods)

General nature, method, mechanism and synthetic applications of the following reactions:

(i) Arndt-Eistert synthesis
(ii) Dakin reaction
(iii) Darzen's glycidic ester synthesis
(iv) Leuckart reaction
(v) Michael reaction
(vi) Willgerodt reaction
(vii) Reimer-Tiemann reaction
(viii) Wittig reaction
(ix) Vilsmeier-Hack reaction
(x) Hell-Volhard-Zelinski reaction
(xi) Ulmann reaction
(xii) Pechmann condensation.

UNIT-II: SUBSTITUTION AND ELIMINATION REACTIONS (15 Periods)

Aliphatic Nucleophilic Substitution:
The SN¹, SN², mixed SN¹ and SN², SET mechanisms. Reactions of Allylic halides, the neighbouring group mechanism, neighbouring group participation by -OH, -NH₂, -COO⁻, RS, halogen, π-bond, aromatic ring, ethereal oxygen.

Aromatic Nucleophilic Substitution:
The SN², SN¹, benzyne and SRN¹ mechanisms, Reactivity - effect of substrate structure, leaving group and attaching nucleophile, The Von Richter, Sommelet-Hauser and Smiles rearrangement.

UNIT-III: STRUCTURE-REACTIVITY PRINCIPLES (15 Periods)

Types of mechanisms, thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammonds postulate, Curtian-Hammet principle, potential energy diagrams, transition state and intermediates, methods of determining mechanisms, isotope effect.

Effect of structure on reactivity - resonance and field effect, steric effect, quantitative treatment. The Hammet equation and linear free energy relationships, substituent and reaction constants, positive and negative deviation from Hammet equation, Taft equation, Solvent effect.
Reference Books:

1. Comprehensive Organic Chemistry by Barton and Ollis (Eds.) (Pergamon Press, 1979), Volume 1: Chapters 2, 7 and 2.8, Volume 2, Chapter 6.6).
6. Carbenes, Benzynes and Nitrenes by Gilchrist, T. L. and Rees.
15. An Introduction to the Chemistry of Carbohydrates by Guthrie and Honeyman [Clarendon Press, 1964, (2/e)].
37. Pericyclic Reactions, S. M. Mukherji, Macmillan India.
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PAPER-III (PHYSICAL CHEMISTRY)

Max. Marks: 60 ( External – 42 + Internal – 18 )                                      Total Periods: 45

SEMESTER-I

UNIT-I: POLYMER CHEMISTRY (15 Periods)
Types of polymers, Stereochemistry of polymers, Mechanism of polymerization (free radical, anionic and cationic), Kinetics of free radical polymerization, Thermodynamics of polymerization, Phase techniques of polymerization (Bulk, solution, suspension and emulsion), Number & mass average molecular mass, Molecular mass determination (Osmometry and Viscometry), Thermal transitions in polymer: glass transition temperature and its significance, Numericals

UNIT-II: CHEMICAL KINETICS (15 Periods)
Collision theory of reaction rates, steric factor, activated complex theory, ionic reactions, Factors affecting reaction rates in solution. Effect of ionic strength on the rate constant.

UNIT- III : THERMODYNAMICS (15 Periods)
Brief resume of concepts of laws of thermodynamics, free energy and entropy, Partial molar properties: Partial molar free energy, Partial molar volume, Partial molar heat content, Chemical Potential, and their significances, determination of these quantities.
Non-ideal systems: Basic idea on Excess functions of non-ideal solutions
Thermodynamic probability and most probable distribution, Boltzmann Distribution law, Partition function and its significance, Rotational, Vibrational & translational: Relation between Partition function and entropy. Partition function and equilibrium constant, Partition function and heat content, Numericals.
UNIT-I: ELECTROCHEMISTRY
Debye-Huckel theory of interionic attraction (qualitative account only), relaxation effect and electrophoretic effect. Ionic strength, Activity coefficient and its determination by solubility and EMF method. Dissociation constant, relation between thermodynamic dissociation constant and dissociation function. Determination of dissociation constant of monobasic acid by conductance method and approximate EMF method, Numericals.
Electrolytic polarization, Decomposition potential, over voltage, concentration polarization, Measurement of over voltage, influence of current density and temperature on over voltage, Ionic discharge as the slow process at cathodes. Tafel and proton transfer theory of hydrogen over voltage, Numericals.

UNIT-I I: MOLECULAR SPECTROSCOPY
Molecular spectra, microwave spectroscopy (Rotational spectroscopy), selection rule for rotational spectra, frequency of rotational spectral lines, vibrational spectra of diatomic molecule, isotopic effect in molecular spectra, harmonic vibration, potential energy, force constant, amplitude of vibration, Anharmonic vibration, Morse potential energy. Numericals.

UNIT-III: SURFACE & COLLOID CHEMISTRY
Surface active agents, classification of Surface active agents, micellization, hydrophobic interaction, critical micellar concentration (CMC), factors affecting the CMC of surfactants, Krafft point and cloud point, counter ion binding to micelles, thermodynamics of micellization-mass action and phase separation model, solubilization, microemulsion, reverse micelles.
Gibbs adsorption isotherms and the determination of surface area/molecule, estimation of surface area of adsorbents (BET equation), surface films on liquids, electrical double layer, Zeta potential and its determination by electrophoresis, Effect of salt on zeta potential, DLVO theory of colloid stability, catalytic activity at surfaces.
Reference Books:
5) Principles of Polymer Science P. Bahadur and N. V. Sastry, Narosa 2006,
6) Mathematics for Chemistry, Doggett and Suctiffe, Longman.
7) Mathematical preparation for Physical Chemistry, F. Daniels, McGraw Hill
10) Basic Chemical Kinetics by G. L. Agrawal
13) Thermodynamics of Chemist, Glasstone, Van Nostrand Co.
17) Textbook of Polymer Science by Billmeyer Wiley.
18) Quantum Chemistry including Spectroscopy by B. K. Sen.
20) Introduction to Molecular Spectroscopy, G. M. Barrow, McGraw – Hill.
22) Basic Principles of Spectroscopy, R. Chang, McGraw-Hill.
25) Introduction to Colloid and Surface Chemistry by Shaw.
26) Physical Chemistry by Protuon and Marron.
27) Statistical Thermodynamics by Gupta M.C.
29) Introduction to Electrochemistry by Glasstone.
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PAPER-IV (INSTRUMENTAL & CHEMICAL ANALYSIS)

Max. Marks: 60 (External – 42 + Internal – 18) Total Periods: 45

SEMESTER-I

UNIT-I: SPECTROSCOPY: UV-Vis and IR (15 Periods)

UV-Visible Spectrophotometry:

IR Spectrophotometry:

UNIT-II: CHROMATOGRAPHY, TLC and GC (15 Periods)

Thin-Layer Chromatography: Selection of stationary and mobile phase – Detection techniques – Elementary idea of HPTLC.


UNIT-III: CHEMICAL MATHEMATICS (15 Periods)

Errors in Chemical analysis, classification of errors, nature and origin of errors, Propagation of error, Accuracy and precision, Average deviation and standard deviation and its physical significance, Normal Distribution curve and its properties. Confidence limit and probability, Statistical treatment for error analysis, student’t’ test, rejection criteria and Q test, method of least square.

UNIT-I I: SUPRAMOLECULAR CHEMISTRY and NANOTECHNOLOGY (15 Periods)

Introduction to nanotechnology: Terminology like soft (condensed) matter, complex fluids Nanoparticles: Synthesis (top down and bottom up approach), Block copolymer nanoaggregates as templates for nanoparticle fabrication, Characterization, properties and applications of nanoparticles.

Introduction to Supramolecules: Host guest chemistry involving crown ethers, cyclodextrins and calixarenes, molecular recognition.

UNIT-III: GREEN CHEMISTRY (15 Periods)

Introduction: Twelve principles of Green chemistry, Atom economy and Waste minimization.

Green solvents and their applications: Ionic liquids, types, properties and applications, ILs as solvents, Supercritical fluids, Supercritical CO₂, its properties and applications in dry cleaning and decaffeination of coffee.

Microwave assisted synthesis: Mechanism and advantages with some examples, Biobased materials: Basic idea on Biopesticides, Biodegradable polymers.

Aqueous phase reaction:
1. Baeyer-Villiger Oxidation
2. Claisen-Schmidt Reaction
3. Diels-Alder reaction
4. Knoevenagel Condensation

Green approach in the synthesis of:
1. Adipic acid
2. Methyl methacrylate
3. Catechol
4. Paracetamol
Reference Books:
   Barrow, McGraw – Hill.
6. Modern Methods of Chemical Analysis (2nd ed.), Pecsok, Shields, Cairns & McWilliam,
   John Wiley & Sons.
13. Instrumental Methods of Analysis by G. W. Ewing.
14. Modern Method of Chemical Analysis by Pecsok, Shield, Cairns, McWilliam, John
    Wiley and Sons.
    1993.
    Delhi-110 002, 1978).
18. Organic Chemistry (3/e) by J. B. Hendrickson, Donald J. Crem and George S. Rammond
    Sons: New York.
20. Green chemistry by V. K. Ahluwalia, Narosa Pub New Delhi
    University Press, 2000, New York, USA.
22. Green Chemistry: An Introductory Text, Mike Lancaster, Green Chemistry Network,
    University of York, RSC, 2002.
VEER NARMAD SOUTH GUJARAT UNIVERSITY, SURAT.
M.Sc. Part-I, CHEMISTRY PRACTICAL SYLLABUS
Marks: 37 [External-26 + Internal-11]

SEMESTER - I

GROUP-A (ORGANIC)
Separation and identification of components in a mixture containing three components (Candidate will prepare two derivatives. Each student should carry out 8 separations)
Separation of organic compounds using paper chromatography technique.

GROUP-B (INORGANIC)
Inorganic Qualitative Analysis (IQA). (One Rare Element)
Spot test detection of Rare Earth metal ion.
Inorganic Preparation.

GROUP-C (PHYSICAL)
1. Determine the dissociation constant of a given monobasic acid pH-metrically.
2. Determine the amount of ferrous sulphate/ferrous ammonium sulphate in given flask potentiometrically using ceric salt solution.
3. Verification of Onsager’s equation and determination of equivalent conductance at infinite dilution of strong electrolytes.
4. Determine the CMC of a surfactant by conductivity measurements.
5. Calculate the molar absorptivity of each of the given two solutions (A) and (B) and also find out concentration of supplied unknown solution colorimetrically.
6. Investigation the reaction between K$_2$S$_2$O$_8$ and KI at two different temperatures and calculate the energy of activation for the reaction.
7. To study the phase diagram of a three component system Water – acetic acid – chloroform.
8. Determination of CMC and area per molecule of a surfactant by surface tension measurement.
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SEMESTER -II

GROUP – A (ORGANIC)
Preparation of the following organic compounds involving not more than two steps (Minimum 5):
(i) Resacetophenone from resorcinol
(ii) m-Nitroaniline from nitrobenzene
(iii) p-Nitroaniline from acetanilide
(iv) p-Bromoaniline from acetanilide
(v) 3-Resorcylic acid from resorcinol
(vi) Benzimidazole from o-phenylene diamine
(vii) Acid Orange-II from sulphanilic acid
(viii) 4-Methyl 7-hydroxy coumarin from resorcinol

Organic Estimations (ANY THREE)
(i) To determine the amount of carboxylic acid and amide in mixture of carboxylic acid and amide.
(ii) To determine the amount of ester and acid in a mixture of ester and acid.
(iii) Determination of molecular weight by Rast's method
(iv) Estimation of Formaldehyde
(v) Amine by bromination

GROUP – B (INORGANIC)
Inorganic Gravimetric Estimations.
Inorganic Volumetric Estimations.

GROUP – C (PHYSICAL)
1. Determine the dissociation constant of a given dibasic acid pH-metrically.
2. Determine the velocity constant of the hydrolysis of ethyl acetate with sodium hydroxide at room temperature by conductance measurements.
3. Determine the solubility of silver chloride in water potentiometrically.
4. To determine the concentration of given components in a mixture colorimetrically.
5. Determine the equilibrium constant of the reaction $\Gamma^+ + I_2 = I_3^-$ by distribution method.
6. Investigation the reaction between $H_2O_2$ and HI at two different temperatures and calculate the energy of activation for the reaction
7. Determine the formula of a complex between $Cu_2^+$ and $NH_3$ by distribution method.
   $Cu^{2+} + nNH_3 = [Cu(NH_3)_n]^{2+}$
8. Determine the molecular weight of a given polymer from viscosity measurement.