VEER NARMAD SOUTH GUJARAT UNIVERSITY
M.Sc.-I (CHEMISTRY)
TO COME IN FORCE FROM JUNE-2008
PAPER-I (INORGANIC CHEMISTRY)

Max. Marks: 52                                                     Total Periods: 90

SECTION-I

UNIT-I    : QUANTUM CHEMISTRY:          (15 Periods)

Operators:

- Definitions
- Operator algebra
- Linear operator
- Hamiltonian operator
- Hermitian operators
- Eigen value relation, and
- Some important theorems

Mechanics:
Angular momentum, Angular momentum operators, Commutation relationship, Eigen values and eigen functions of angular momentum, Shift operators, electron spin, coupling of angular momentum,

- Simple harmonic oscillator (where the potential energy is not constant)
- One dimensional harmonic oscillator
- Normalisation and the characteristic of the eigen functions of a harmonic oscillator.
- The selection rule for the harmonic oscillator.
- The two particle rigid rotator.
- Moment of inertia, Derivation of kinetic energy of relation, Selection rule.

Reference Books:


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\(_2\)\(_v\), D\(_2\)h, C\(_3\)\(_v\) and D\(_3\)h point groups.
Application of group theory to -
- Transformation properties of atomic crystals.
- Hybridisation scheme for $\sigma$ and $\pi$-bonding.
- Spectroscopy.

Reference Books:

UNIT-III : The reaction rates and mechanism of Inorganic reactions (15 Periods) of transition metal complexes (Inorganic Reaction Mechanism):

(a) **Introduction (What is kinetics?):**
Labile and inert complexes, factors responsible for lability and inertness of complexes.

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

**Fast reaction techniques:**
(a) The constant flow method
(b) The stopped flow method
(c) The quenched flow method
(d) Electrochemical techniques
(e) Nuclear and paramagnetic resonance
(f) Relaxation techniques.

(c) **The interpretation of rate data:**
(i) Reaction order and rate constants
(ii) The effect of temperature
(iii) The effect of ionic strength
(iv) Isotopic labeling

(d) **Solvolytic reaction:**
(i) Importance of the solvent
(ii) Isotopic exchange between complex and the solvent
(iii) The hydrolysis of complexes

(e) **Substitution reactions:**
(i) Kinetic features of substitution reactions
(ii) Rates of non-isotopic ligand replacement
   (A) Four coordinated complexes (Pt$^{2+}$, Pd$^{2+}$ complexes)
   Trans effect, Trans effect theories.
   (B) Six coordinated complexes (Co$^{3+}$ and Cr$^{3+}$ complexes)

(f) **Oxidation-Reduction processes.**
Reference Books:

SECTION-II

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

(I) Introduction:
   (i) Definitions of magnetic properties
   (ii) Types of magnetic bodies
   (iii) The source of paramagnetism
   (iv) Diamagnetism and Pascal's constant

(II) The Elementary theory of magnetochemistry.

(III) Properties of paramagnetic bodies:
   (i) Thermal energy and magnetic property
   (ii) Magnetic moments of different multiplate width

(IV) Experimental:
   (i) Determination of magnetic susceptibility: (a) Gouy method, and
       (b) Faraday method.
   (ii) Magnetic anisotropy.

(V) Magnetic properties based on crystal field model.

(VI) Numerical Problems on Magnetic Property.


(VIII) Antiferromagnetism and Ferromagnetism:
   (i) Types of antiferromagnetic interaction.
   (ii) Antiferromagnetic exchange pathways.

Reference Books:
UNIT-V : METAL π-COMPLEXES: (15 Periods)

Metal carbonyls, structure and bonding, vibrational spectra of metal for bonding and structural elucidation, important reactions of metal carbonyls.
Bonding, structure and important reactions of transition metal nitrosyl, dinitrogen and dioxygen complexes; (Two Compounds VIZ ) tertiary phosphine as ligand.

UNIT-VI : INORGANIC POLYMERS: (15 Periods)

(1) Introduction:
- Definition of polymers and their depiction.
- Types of characteristic of inorganic polymers.

(2) Characterization of inorganic polymers (Physical properties)
- By molecular weights
  - number average
  - weight average
- Experimental techniques determination of molecules weight of polymers by
  - a chemical method
  - light scattering
- Uses of molecular weights
- 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
  - Dilatometry, crystallography, spectroscopy and colorimetry, some additional information from X-ray diffraction.

Transition: (Property w.r. to temperature)
- Definitions
- Illustrative representations
- Diilatometric results
- Calorimetric results
  - Pomb calorimetry
  - DTA
  - DSC

Mechanical properties
- Elasticity
- Viscosity
- Viscoelasticity
Classification, types of inorganic polymers, synthesis, properties, structures and uses in following polymers:
(i) Polyphosphazenes
(ii) polysiloxanes

Reference Books:

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SECTION-I

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

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

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

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

(ii) **Carbanions:**

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

(iii) **Carbenes:**

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

(iv) **Free Radicals:**

Types of free radical reactions, free radical substitution mechanism, mechanism at
aromatic substrate, neighbouring group assistance. Reactivity for aliphatic and aromatic
substrates at bridge-head.

Reactivity in attacking radicals. The effect of solvents on reactivity. 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.

(v) **Nitrenes:**

Mechanism of Hofmann, Curtius, Lossan and Schmidt rearrangement.

(vi) **Arynes:**

Methods of generation, Reactions and structure.

Recommended 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).
2. Reaction Mechanism and Reagents in Organic Chemistry by C. R. Chatwal (Himalaya
3. Organic Chemistry Reactions and Reagents by O. P. Agrawal (Goel Publishing House, Meerut,
   1986).
4. The Chemistry of Free Radicals by R. L. Hudang, S. H. Goh and S. H. Ong (Edward Arnold,
   1974).
6. Carbenes, Benzynes and Nitrenes by Gilchrist, T. L. and Rees.
UNIT-II : GREEN CHEMISTRY AND PHOTOCHEMISTRY (15 Periods)

(A) BASIC PRINCIPAL OF GREEN CHEMISTRY

TWELVE PRINCIPLES:

Prevention of Waste / By – products, Maximum incorporation of the reactants into the final products, Prevention or minimization of hazardous products, Designing safer chemicals, Energy requirements for synthesis, Selection of starting materials, Use of protecting groups, Use of catalyst, products designed should be biodegradable, Designing of manufacturing plants, Strengthening of analytical techniques.


(B) ORGANIC PHOTOCHEMISTRY:

(i) Photochemical Reactions:


(ii) Photochemistry of Carbonyl Compounds:


Recommended Books:


UNIT-III : (15 Periods)

(A) CARBOHYDRATES:

Structural determination of starch and cellulose, their conformations Carbohydrate metabolism - Kreb's cycle, glycolysis, glycogenesis and glycojenolysis, glyconeogenesis,

(B) NUCLEIC ACID:

Purine and pyrimidine bases of nucleic acids, base pairing via H-bonding. Chemical and enzymatic hydrolysis of nucleic acids, structure of nucleosides, nucleotides, chemical synthesis of nucleosides. Structure of Ribonucleic acid (RNA) and deoxyribonucleic acid (DNA). The chemical basis for heredity, an overview of replication of DNA, transcription, translation and genetic code - Chemical synthesis of ADP, ATP.
Recommended Books:

4. An Introduction to the Chemistry of Carbohydrates by Guthrie and Honeyman [Clarendon Press, 1964, (2/e)].

SECTION-II

UNIT-IV : (15 Periods)

(A) ORGANOMETALLIC COMPOUNDS:
Carbon-metal bonds in organometallic compounds, organometallic nomenclature, Preparations of organolithium, Organocopper and lithium diorganocuprate and their synthetic applications.
Preparation of organoboranes, stereochemistry of hydroboration, mechanism of hydroboration - oxidation, synthetic uses of organozinc compounds.

Addition to Carbon-Hetero multiple bonds:
Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acids, esters and nitriles.

Recommended Books:


(B) EMERGING GREENER TECHNOLOGIES AND ALTERNATIVE ENERGY SOURCES:

- Chemistry using Microwaves:
  (a) Microwave heating
  (b) Microwave assisted Reactions
- Sonochemistry:
  (a) Sonochemistry and green chemistry
- Photochemical reactions:
  (a) Advantages and challenges faced by Photochemical Processes.
  (b) Example of Photochemical Reactions

Recommended Books:

UNIT-V : HETEROCYCLIC CHEMISTRY: (15 Periods)

(1) Nomenclature of Heterocycles:
Replacement and systematic nomenclature for monocyclic and fused heterocycles and bridged heterocycles.

(2) Aromatic Heterocycles and Heterocyclic Synthesis:
General chemical behaviour of aromatic heterocycles, Classification of heterocyclic compounds, Principles of heterocyclic synthesis involving cyclization reactions and reactivity and tautomerism of aromatic, heterocyclic compounds and their mechanism containing two heteroatoms (O, S and N) and their condensed systems.

(3) Five-membered and Benzo fused Five-membered Heterocycles:
Oxazole, Isoxazole, Thiazole, Isothiazole, Pyrazole, Imidazole, Benzoxazole, Benzthiazole, Benzopyrazole, Benzimidazole.

(4) Six-membered and Benzo fused six-membered heterocycles with two heteroatoms:
Pyridazine, pyrimidine, pyrazine, cinnoline, quinoxaline, quinazoline, morpholine, phenoxazine, naphthyridine - phenothiazine, phenazine.

Recommended Books:
6. Ring Index by Patterson, Capell and Walker (American Chemical Society, New York, 1960).

UNIT-VI : STEREOCHEMISTRY AND CONFORMATIONAL ANALYSIS: (15 periods)

Concept of isomerism, Dynamic stereochemistry, prochiral relationships, Resolution of racemic modifications. Optical activity in the absence of chiral carbon (biphenyls, allenes and spiranes), Chirality due to helical shape.
Conformational analysis of cyclohexanes, Decalins, perhydro-phenanthrins. Heterocyclic compounds (only comparison with carbo-cyclic compounds).

More Reference Books Recommended:
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M.Sc.-I (CHEMISTRY)
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PAPER-III (PHYSICAL CHEMISTRY)

Max. Marks: 52

SECTION-I

UNIT I

(A) POLYMER CHEMISTRY
Types of polymers, Stereochemistry of polymers, Mechanism of polymerization (free radical, anionic and cationic), Kinetics of free radical polymerization Number & mass average molecular mass, Molecular mass distribution, Practical significance of molecular mass, Molecular mass determination (Osmometry and Viscometry), Numericals

(B) CHEMICAL MATHEMATICS
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, Review of basics of differential and integral calculus.

UNIT II

CHEMICAL KINETICS
Collision theory of reaction rates, steric factor, activated complex theory, ionic reactions, Factors affecting reaction rates in solution. Effect of solvent and ionic strength (primary salt effect) on the rate constant, secondary salt effects.

UNIT III

(A) CLASSICAL THERMODYNAMICS
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: Excess functions of non-ideal solutions

(B) STATISTICAL THERMODYNAMICS
Thermodynamic probability and most probable distribution, Boltzmann Distribution law, Bose-Einstein and Fermi-Dirac statistics, partition function and its significance, Rotational, Vibrational & Electronic partition functions for diatomic molecules. Partition function and Thermodynamic function. (Boltzmann-Planck’s equation, partition function & heat content, partition function & Gibb’s free energy, partition function and third law of thermodynamics. Numericals.

SECTION-II

UNIT IV

(A) ELECTROLYTES IN SOLUTIONS
Debye-Huckel theory of interionic attraction (qualitative account only), relaxation effect and electrophoretic effect, Activity, activity coefficient, mean activity coefficient, activity in electrolytic solutions- relaxation between concentration and activity. Ionic strength, Determination of activity coefficient (solubility and EMF method). Dissociation constant, relation between thermodynamic

(B) OVER VOLTAGE
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. Processes at cathodes-Metal deposition. Numericals.

UNIT V

(A) 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.

(B) NUCLEAR CHEMISTRY

UNIT VI

(A) MICELLES
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-phase separation model, solubilization, micro emulsion, reverse micelles.

(B) ADSORPTION/ COLLOIDS
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, electro-kinetic phenomenon, Zeta potential and its determination by electrophoresis, Effect of salt on zeta potential, DLVO theory of colloid stability catalytic activity at surfaces, Numerical.

Books Recommended:
5) Principles of Polymer Science P Bahadur and NV Sastry Narosa 2006,
6) Mathematics for Chemistry, Doggett and Sucliffe , 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.
18) Textbook of Polymer Science by Billmeyer Wiley.
19) Quantum Chemistry including Spectroscopy by B.K.Sen.
26) Introduction to Colloid and Surface Chemistry by Shaw.
27) Physical Chemistry by Protuonand Marron.
28) Statistical Thermodynamics by Gupta M.C.
30) Introduction to Electrochemistry by Glasstone.