VEER NARMAD SOUTH GUJARAT UNIVERSITY

M.Sc. PART-I

CHEMISTRY

TO COME IN FORCE FROM JUNE-2002
PAPER-I (INORGANIC)

Max. Marks: 75 (External-52 + Internal-23) Total Periods: 90

UNIT-I : QUANTUM CHEMISTRY: (15 Periods)

- **Operators :** - Definitions
- Operator algebra
- Linear operator
- Hamiltenian 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, particle on a sphere.

  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:

1. Quantum Chemistry by Ira N. Levine, Prentice-Hall of India Pvt. Ltd., New Delhi, 1994.
2. Introductory Quantum Chemistry (Third edition) by A. K. Chandra Tata McGraw Hill Pub. Co. Ltd., New Delhi, 1988.
3. Quantum Mechanics in Chemistry (3rd edition) by N. W. Hanna, Benjamin, Menlo Park, Calif, 1981.
4. Problems in Quantum Chemistry and Physics by C. S. Johnson and L. G. Pedersen, Addison-Wesley, Reading, Mass., 1974.
5. Problems in Quantum Chemistry by P. Jorgensenand J. Oddershede Addison-Wesley, Reading, Mass., 1983.
6. Quantum Chemistry and Spectroscopy by M. S. Pathania, Vishal Publications, India, 1981.

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

(I) Representation of groups:

(i) Preparation of matrices and vectors.
(ii) Matrix notations for geometrical transformations.
(iii) Orthogonality theorem and its consequences.
(iv) Reducible and irreducible representations and their relation.
(v) Preparation of character table for 2v, D_2h, C_3v and D_3h point groups.

(II) Application of group theory to -

(i) Transformation properties of atomic crystals.
(ii) Hybridisation scheme for σ and π-bonding.
(iii) Spectroscopy.

Reference Books:

1. Chemical applications of group theory by F. A. Cotton (Second edition), Wiley Eastern Limited, 1976, New Delhi.

2. Group theory and its applications by P. K. Bhattacharya, Himalaya Publishing House, Mumbai, 1986.

3. Group theory and symmetry in Chemistry by L. R. Hall, McGraw Hill, New York, 1989.

4. Quantum Chemistry by I.N. Levine (4^{th} edition), Prentice-Hall, New Delhi, 1994.

5. Introductory Quantum Chemistry by A. K. Chandra (4^{th} edition), Tata McGraw Hill Pub. Co. Ltd., New Delhi.

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

(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 resenonance
(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 labelling

(d) Solvolytic reaction:

(i) Importance of the solvent
(ii) Isotopic exchange between complex and the solvent
(iii) The effect of 'inert' ions.
(iv) 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:

1. 'Kinetics and Mechanism' by A. A. Frost and R. G. Pearson, Wiley, New York, 1953, 1961.

2. Mechanism of Inorganic Reactions by F. Basolo and R. G. Pearson, Second Edition, Wiley Eastern Limited, New Delhi, 1977.

3. Advanced Inorganic Chemistry and Radiochemistry, H. Taube, 1, 2 (1959), Review article. Inorganic Reaction Mechanism by S. G. Skyes.

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

(I) Introduction:

(i) Definations of magnetic properties
(ii) Types of magnetic bodies
(iii) The source of paramagnetism
(iv) Diamagnetismand Pascal's constant

(II) The leementary 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) Van Vleck equation: (I) Derivation of the Van Vleck equation.

(VII) Magnetic moment - (I) intrinsic orbital contribution, (ii) Spin orbit coupling, and (iii) Temperature independent paramagnetism (T.I.P.). Anamalous magnetic moments, magnetic exchange coupling and spin cross over.

(VIII) Antiferromagnetism and Ferromagnetism:

- (i) Types of antiferromagnetic interaction.
- (ii) Antiferromagnetic exchange pathways.

Reference Books:

1. Magnetochemistry by R. L. Carlin.
2. Introduction to Magnetochemistry by A. Carnshaw, Academic Press, London.
3. Magnetism and Transition Metal Complexes by F. E. Mabb and D. J. Machin, Chapman and Hall, London.
4. Advanced Inorganic Chemistry by F. A. Cotton and R. G. Wilkinson, John Wiley & Sons, N.Y.
5. Elements of Magnetochemistry by A. Syamal and R. L. Dutta, Affiliated East-West Press, New Delhi, 1993.

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, preparation, bonding, structure and important reactions of transition metal nitrosyl, dinitrogen and dioxygen complexes; 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
  - viscometry
- 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
- Characterisation of crystallinity
  - intermolecular and intramolecular
- Methods for determining percent crystallinity
  - Dilatometry, crystallography, spectroscopy and colorimetry, some additional information from X-ray diffraction.

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

(4) Mechanical properties
- Elasticity
- Viscosity
- Viscoelasticity

(5) Classification, types of inorganic polymers, synthesis, properties, structures and uses in following polymers:

(i) Polyphosphazenes
(ii) Polysilanes and polysiloxanes
(iii) Coordination polymers

Reference Books:

(1) Inorganic Polymers by James E. Mark, H. R. Allcock and Robert West, Prentice Hall of India Pvt. Ltd., New Delhi, 1992.

(2) Text-book of Polymer Science, 2nd edition, by F. W. Jr. Billmeyer Jr., Wiley-Interscience, New York, 1971.

(3) Inorganic and Organometallic Polymers by M. Zelding, K. J. Wynne and H. R. Allcock, ACS Symposium Series, American Chemical Society, Washington, DC, Vol. 360 (1988).

(4) Introductory Polymer Chemistry by G. S. Mistra, Wiley Eastern Ltd., 1993.

(5) Phosphorous-Nitrogen Compounds, H. R. Allcock, Academic, New York, 1972.

(6) In Encyclopaedia of Polymer Science and Engineering, 2nd edn., by R. Baney and G. Chandra, Wiley-Interscience, New York, 1987.

VEER NARMAD SOUTH GUJARAT UNIVERSITY

M.Sc. PART-I

CHEMISTRY

TO COME IN FORCE FROM JUNE-2002

PAPER-II (ORGANIC)

Max. Marks: 75 (External-52 + Internal-23) Total Periods: 90

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, Reiner-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, Losson 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 Publishing House, Bombay, 1987).
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).
5. Principles of Ionic Organic Reagents by E. R. Alexander (John Wiley & Sons, Inc.).
6. Carbenes, Benzynes and Nitrenes by Gilchrist, T. L. and Rees.
7. Advance Organic Chemistry by Jeery March Principles.

UNIT-II : ORGANIC PHOTOCHEMISTRY: (15 Periods)

(i) Photochemical Reactions:

Photochemical energy, Electronic excitation and molecular, Orbital view of excitation. Excited states and modes of dissipation of energy. Energy transfer, quantum efficiency.

(ii) Photochemistry of Carbonyl Compounds:

Reactivity of electronically excited ketones. Representation of excited states of ketones, Photoreduction. Norrish Type I & II reactions. Reactions of cyclic ketones, Oxetane formation (Paterno-Buchi reaction).

(iii) Photochemistry of Olefines:

Cis-trans isomerisations, Dimerisation reactions, Photochemistry of conjugated olefins.

Recommended Books:

1. Reaction Mechanism in Organic Chemistry by S. M. Mukherji and S. P. Singh (McMillan India Ltd., 1976).
2. Molecular Reactions and Photochemistry by Charles H. Depuy and Orville L. Chapman (Prentice Hall of India Pvt. Ltd., 1975).
3. Fundamentals of Photochemistry by K. K. Rohatgi-Mukherjee (Eastern Limited, New Delhi-110 002, 1978).
4. Organic Chemistry (3/e) by J. B. Hendrickson, Donald J. Crem and George S. Rammond (McGraw-Hill Book Co. & Kogekusha Co. Ltd., 1970).

UNIT-III : CARBOHYDRATES AND NUCLEIC ACID: (15 Periods)

(A) Structural determination of starch and cellulose, their conformations

Carbohydrate metabolism - Kreb's cycle, glycolysis, glycogenesis and glycogenolysis, glyconeogenesis, pentose phosphate pathway.

(B) 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:

1. Organic Chemistry by Finar, I. L., Vol. II (5/e) (London, ELBS).
2. Organic Chemistry (5/e) by Morrison & Boyd (Prentice Hall).
3. The Carbohydrates by S.F. Dyke, Volume V in the series, 'The Chemistry of Natural Products', edited by K. W. Bentley (Interscience Publishers).
4. An Introduction to the Chemistry of Carbohydrates by Guthrie and Honeyman [Clarendon Press, 1964, (2/e)].
5. A guide to IUPAC nomenclature of Organic Compounds, R. Fanico, W. R. Powell and Jean-Claude Richard, Jain Interscience Press, New Delhi, 5-d Kamala Nagar.

UNIT-IV : ORGANOMETALLIC COMPOUNDS: (15 Periods)

(A) 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.

(B) Addition to Carbon-Hetero multiple bonds:

Mechanism of metal hydrige reduction of saturated and unsaturated carbonyl compounds, acids, esters and nitriles.

Recommended Books:

1. Advanced Organic Chemistry (2/e) Part by Carey, F. A. and Sundberg R. J. (Plenum Publishing Corporation, 1984).
2. Organic Chemistry by Francis A. Carey (McGraw-Hill Book Co., 1987).
3. Principles of Organic Chemistry by R.C.C. Norman (Chapman and Hall, 1986).

4. Organometallic Chemistry by P. L. Pauson (Edward Arnold, 1968).
5. Principles of Organometallic Chemistry by Coats, Green, Powell & Wade (Chapman and Hall, 1977).
6. Guide Book to Organic Synthesis by R. K. Mackie & D. M. Smith (Longman, 1983).
7. Organic Synthesis via Poranos by H. C. Brown (John Wiley & Sons, New York, 1975).

UNIT-V : HETEROCYCLIC CHEMISTRY: (15 Periods)

(1) Nomenclature of Heterocycles:

Replacement and systematic nomenclature for monocyclic, fused 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, Isooxazole, Thiazole, Isothiazole, Pyrazole, Imidazole, Benzooxazole, Benzothiazole, Benzopyrazole, Benzoimidazole.

(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:

1. Chemistry of Heterocyclic Compounds by Badger (Academic Press, 1963).
2. Heterocyclic Compounds by R. C. Elderfield (Ed.), Vol. 1-9 (Wiley, New York, 1960-65).
3. An Introduction to the Chemistry of Heterocyclic Compounds by R. M. Acheson (John Wiley & Sons Ltd., New York, 1967).
4. Heterocyclic Chemistry (2/e) by J. A. Joule and G. F. Smith (Van Nostrand Reinhold (UK) Co. Ltd., 1978).
5. The Chemistry of Carbon Compounds by Rodd, E. R. (Ed.), Vol. 4A to 4C (Elsevier, Amsterdam, 1957-1973).
6. Ring Index by Patterson, Capell and Walker (American Chemical Society, New York, 1960).

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

(A) Concept of isomerism, Dynamic stereochemistry, prochiral relationships, Resolution of rascemic modifications. Optical activity in the absence of chiral carbon (biphenyls, allenes and spiranes), Chirality due to helical shape.

(B) Conformational Analysis:

Conformational analysis of cyclohexanes, Decalins, perhydro-phenanthrins. Heterocyclic compounds (only comparison with carbo-cyclic compounds).

Recommended Books:

1. Advanced Organic Chemistry by Carey & Sundberg (3^{rd} edition).
2. Organic Chemistry by I. L. Finar, Volume II (Sixth edition).

More Reference Books Recommended:

1. Advanced Organic Chemistry-Reactions, Mechanismand Structure, Jerry March, John Wiley.
2. Advanced Organic Chemistry, (Vol. A & B), F. A. Carey and R. J. Sundberg, Plenum.
3. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman.
4. Structure and Mechanism in Organic Chemistry, C. K. Ingold, Cornell University Press.
5. Organic Chemistry, R. T. Morrison and R. N. Boyd, Prentice-Hall.
6. Modern Organic Reactions, H. O. House, Benjamin.
7. Principles of Organic Synthesis, R.O.C. Norman and J. M. Coxon, Blackie Academic and Professional.
8. Pericyclic Reactions, S. M. Mukherji, Macmillan, India.
9. Reaction Mechanism in Organic Chemistry, S. M. Mukherji and S. P. Singh, Macmillan.
10. Stereochemistry of Organic Compounds, D. Nasipuri, New Age International.
11. Stereochemistry of Organic Compounds, P. S. Kalsi, New Age International.s

VEER NARMAD SOUTH GUJARAT UNIVERSITY

SYLLABUS FOR M.Sc. PART-I (PHYSICAL) CHEMISTRY
TO COME IN FORCE FROM JUNE-2002 (Revised)
PAPER-III (PHYSICAL)

Max. Marks: 75 (External-52 + Internal-23) Total Periods: 120

UNIT-I : CHEMICAL MATHEMATICS, TREATMENT OF ANALYTICAL DATA AND MACROMOLECULES: (15 Periods)

(A) Calculus:

Functions, Differential calculus: rules for differentiation, application of differential calculus including maxima and minima, exact and inexact differentials with their application to thermodynamic properties.

Integral calculus, basic rules for integration, integration by parts, partial fraction and substitution. applications of integral calculus.

(B) Treatment of Analytical Data Statistically:

The normal error curve, Standard deviations, Student 't' test, confidence interval of the mean, criteria for rejection of an observation, Q test, methods of least square fitting deviation of equations for linear equations

(C) Macromolecules:

Polymer - definition, types of polymers, kinetics of polymerization, mechanism of polymerization. Molecular mass, number and mass average molecular mass, molecular mass determination (osmometry, and viscometry, Average dimensions of various chain structures.

UNIT-II : THERMODYNAMICS: (15 Periods)

Classical Thermodynamics:

Brief resume of concepts of laws of thermodynamics, free energy, chemical potential and entropies. Partial molar properties, partial molar free energy, partial molar volume and partial molar heat content and their significances. Determinations of these quantities.

Non-ideal systems: Excess functions for non-ideal solutions. Thermodynamic excess functions, regular solution, Determination of excess volume, Case study of Ar+Kr, Benzene + cyclohexane, Xylene mixtures, CH3l + CCl4.

(D) Statistical Thermodynamics:

Concept of distribution, thermodynamic probability and most probable distribution. Distribution laws, Baltzman Distribution Law. The partition function and its significant. Partition functions, translational, rotational, vibrational and electronic partition functions. Evaluation of thermodynamic properties in terms of partition functions (Energy and Entropy, Free energy and equilibrium constants).

VEER NARMAD SOUTH GUJARAT UNIVERSITY

SYLLABUS FOR M.Sc. PART-I CHEMISTRY
TO COME IN FORCE FROM JUNE-2002 (Revised)
PAPER-IV (ORGANIC)

Max. Marks:75 (External-54 + Internal-21) Total Periods: 90

UNIT-I : REARRANGEMENTS: (15 Periods)

General mechanistic considerations, Nature of migration, Migratory aptitude, Memory effects in respect of the following:

(A) 1,2-Rearrangements:

(a) Carbon to carbon migrations of R, H and Ar:

(i) Pinacol-Pinacolone rearrangement
(ii) Wagner-Meerwein rearrangement
(iii) The Dienone-Phenol rearrangement
(iv) Demjanov
(v) Acid catalysed rearrangements of aldehydes and ketones
(vi) Benzil-Benzilic acid rearrangement
(vii) Favorskii rearrangement
(viii) Favorskii rearrangement

(b) Carbon to carbon migration of other groups:

(i) Neber rearrangement
(ii) Migrations of halogen, hydroxy, amino etc.

(c) Carbon to oxygen migration of R and Ar:

(i) Baeyer-Villiger rearrangement
(ii) Rearrangement of hydroperoxide

(B) Non 1,2 Rearrangement:

(i) Claisen rearrangement
(ii) Benzidine rearrangement

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

(a) Aliphatic Nucleophilic Substitution:

The SN^i mechanisms. Reactions of Allylic halides, The neighbouring group mechanism, neighbouring group participation by -OH, $-NH_2$, $-COO^-$, -RS, -halogen, π-bond, aromatic ring, etheral oxygen.

(b) Aromatic Nucleophilic Substitution:

The SN^2, SN^1, benzyne and SRN^1 mechanisms, Reactivity - effect of substrate structure, leaving group and attaching nucleophile, The Von Richter, Sommelet-Hauser and Smiles rearrangement.

UNIT-III : 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) Mannich reaction
(vi) Michael reaction
(vii) Willgerodt reaction
(viii) Reimer-Tiemann reaction
(ix) Knoevenagel reaction
(x) Wittig reaction
(xi) Hell-Volhard-Zelinskii reaction
(xii) Vilsmeyer-Hack reaction
(xiii) Oppenauer oxidation
(xiv) Elb's persulphate oxidation

UNIT-IV : PERICYCLIC REACTIONS: (15 Periods)

Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl systems. Classification of pericyclic reactions. Woodward-Hoffmann correlation diagrams. FMO and PMO approach. Electrocyclic reactions - Conrotatory and disrotatory motions, 4n, 4n+2 and allyl systems. Cycloadditions - antrafacial and suprafacial additions, 4n and 4n+2 systems, 2+2 addition of ketenes, 1,3-dipolar cycloadditions and cheleotropic reactions.

Sigmatropic rearrangements - Suprafacial and antarafacial shifts of H.

UNIT-V : NATURE OF BONDING IN ORGANIC MOLECULES AND AROMATICITY: (15 Periods)

Aromaticity and aromatic character, Frost circle diagram for cyclo-butadiene, benzene and others. Concepts of aromaticity resonance and chemical stabilization – aromatic character based on NMR-criteria to check aromaticity character.

Crown ether complexes and cryptands, inclusion compounds, cyclodextrins, catenanes and rotaxanes.

Huckel rule, energy level of π molecular orbitals, Huckel molecular orbitals (HMO) method, orbital symmetry, MO of simple organic systems such as ethene, allyl and butadiene.

Aromaticity in benzenoid and non-benzenoid compounds and charged rings, annulenes, antiaromaticity, homoaromaticity.

UNIV-VI : STRUCTURE-REACTIVITY PRINCIPLES: (15 Periods)

(a) Types of mechanisms, types of reactions, 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, Hard and soft acids and bases.

(b) 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. Advanced Organic Chemistry-Reactions, Mechanism and Strucuture, Jerry March, John Wiley.
2. Advanced Organic Chemistry, F. A. Carey and R. J. Sundberg, Plenum.
3. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman.
4. Structure and Mechanism in Organic Chemistry, C. K. Ingold, Cornell University Press.
5. Organic Chemistry, R. T. Morrison and R. N. Boyd, Prentice-Hall.
6. Modern Organic Reactions, H. O. House, Benjamin.
7. Principles of Organic Synthesis, R.O.C. Norman and J. M. Coxon, Blackie Academic & Professional.
8. Pericyclic Reactions, S. M. Mukherji, Macmillan, India.
9. Reaction Mechanism in Organic Chemistry, S. M. Mukherji and S. P. Singh, Macmillan.
10. Stereochemistry of Organic Compounds, D. Nasipuri, New Age International.
11. Stereochemistry of Organic Compounds, P. S. Kalsi, New Age International.

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M.Sc. PART-I

CHEMISTRY
TO COME IN FORCE FROM JUNE-2002
PAPER-IV (INORGANIC)

Max. Marks: 75 (External-52 + Internal-23) Total Periods: 90

UNIT-I : UNIFYING PRINCIPLES AND MICROWAVE SPECTROSCOPY: (15 Periods)

Electromagnetic radiation, interaction of electromagnetic radiation with matter-absorption, emission, transmission, reflection, refraction, dispersion, polarisation and scattering. Uncertainty relation and natural line width and natural line broadening, transition probability, results of the time dependent perturbation theory, transition moment, selection rules, intensity of spectral lines, Born-Oppenheimer approximation, rotational, vibrational and electronic energy levels.

Classification of molecules, rigid rotor model effect of isotropic substitution on the transition frequencies, intensities, non-rigid rotor. Stark effect, nuclear and electron spin interaction and effect of external field. Applications.

UNIT-II : VIBRATIONAL SPECTROSCOPY: (15 Periods)

(a) Infrared Spectroscopy:

Review of linear harmonic oscillator, vibrational energies of diatomic molecules, zero point energy, force constant and bond strengths; anharmonicity, Morse potential energy diagram, vibration-rotation spectroscopy, P,Q,R branches. Breakdown of Oppenheimer approximat- ion; vibrations of polyatomic molecules. Selection rules, normal modes of vibration, group frequencies, overtones, hot bands, factors affecting the band positions and intensities, far IR region, metal-ligand vibrations, normal co-ordinate analysis.

(b) Raman Spectroscopy:

Classical and quantum theories of Raman effect. Pure rotational, vibrational and vibrational-rotational Raman spectra, selection rules, mutual exclusion principle. Resonance Raman spectroscopy, coherent anti Stokes Raman spectroscopy (CARS).

UNIT-III : ELECTRONIC SPECTROSCOPY: (15 Periods)

(a) Atomic Spectroscopy:

Energies of atomic orbitals, vector representation of momenta and vector coupling, spectra of hydrogen atom and alkali metal atoms.

(b) Molecular Spectroscopy:

Energy levels, molecular orbitals, vibronic transitions, vibrational progressions and geometry of the excited states, Franck-Condon principle, electronic spectra of polyatomic molecules. Emission spectra; radiative and non-radiative decay, internal conversion, spectra of transition metal complexes, charge-transfer spectra.

(c) Photoelectron Spectroscopy:

Basic principles; photo-electric effect, ionization process, Koopman's theorem. Photoelectron spectra of simple molecules, ESCA, chemical information from ESCA. Auger electron spectroscopy - basic idea.

UNIT-IV : MAGNETIC RESONANCE SPECTROSCOPY: (15 Periods)

(a) Nuclear Magnetic Resonance Spectroscopy:

Nuclear spin, nuclear resonance, saturation, shielding of magnetic nuclei, chemical shift and its measurements, factors influencing chemical shift, deshielding, spin-spin interactions, factors influencing coupling constant 'J'. Classification (ABX, AMX, ABC, A_2B_2 etc.), spin decoupling; basic ideas about instrument, NMR studies of nuclei other than proton - ^{13}C, ^{19}F and ^{31}P. FT NMR, advantages of FT NMR, use of NMR in medical diagnostics.

(b) Electron Spin Resonance Spectroscopy:

Basic principles, zero field splitting and Kramer's degeneracy, factors affecting the 'g' value. Isotropic and anisotropic hyperfine coupling constants, spin Hamiltonian, spin densities and McConnell relationship, measurement techniques, applications.

(c) Nuclear Quadrupole Resonance Spectroscopy:

Quadrupole nuclei, quadrupole moments, electric field gradient, coupling constant, splittings. Applications.

UNIT-V : QUANTUM CHEMISTRY: (15 Periods)

(1) Approximate Methods:

- General Time independent perturbation theory
- The application of perturbation method with examples
- The variation theorem
- The application of variation method
- Application of the variation method to other states
- Examples of variation and perturbation calculations.

(2) Electron Spin and Pauli Principle:

- Electron spin
- Spin and the hydrogen atom
- The Pauli principle, The Pauli exclusion principle
- Perturbation treatment of the lithium ground state
- Variation treatments of the lithium ground state
- Spin magnetic moment
- Ladder operators for electron spin

(3) Many electron atoms:

- The Hartree-Fock self consistant filled model
- Orbitals and periodic tables
- Electron correlations
- Addition of angular momenta
- Angular momentum in many electron - The atom Hamiltonian - The Slater rules
- Spin orbit interactions

UNIT-VI : STEREOCHEMISTRY AND BONDING IN MAIN GROUP COMPOUNDS: (15 Periods)

VSEPR, Walsh diagrams (tri- and penta-atomic molecules), dπ-pπ bonds, Bent rule and energetics of hybridisation, some simple reactions of covalently bonded molecules.

Books Suggested:

1. Introduction to Quantum Chemistry, A. K. Chandra, Tata McGraw Hill.
2. Quantum Chemistry, Ira N. Levine, Prentice Hall.
3. Modern Spectroscopy, J. M. Hollas, John Wiley.
4. Applied Electron Spectroscopy for Chemical Analysis, ed. By H. Windawi and F. L. Ho, Wiley Interscience.
5. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, R. V. Parish, Ellis Harwood.
6. Physical Methods in Chemistry, R. S. Drago, Saunders College
7. Chemical Application of Group Theory, F. A. Cotton.
8. Introduction to Molecular Spectroscopy, G. M. Barrow, McGraw Hill.
9. Basic Principles of Spectroscopy, R. Chang, McGraw Hill.
10. Theory and applications of UV Spectroscopy, H. H. Jaffe and M. Orchin, IBM-Oxford.
11. Introduction to Photoelectron Spectroscopy, P. K. Ghosh, John Wiley.
12. Introduction to Magnetic Resonance, A Carrington and A. D. Maclachalan, Harper & Row.

UNIT-III : CHEMICAL DYNAMICS: (15 Periods)

Collision theory of reaction rates, steric factors rate theories based on thermodynamics, conventional transition state theory, derivation of rate equation.

Kinetics and mechanism of following complex reactions in detail - (I) Reversible, (ii) Parallel, (iii) Consecutive, (iv) Chain (thermal and photochemical) and Enzyme reactions. Hydrogen-Bromine, Hydrogen-Chlorine, Hydrogen-iodine, decomposition of nitrogen-pentoxide, Reaction between NO and O_2, Effect of temperature and pH on enzyme reaction.

UNIT-IV : (15 Periods)

(A) Surface and Colloid Chemistry:

Gibbs adsorption isotherm, estimation of surface area (BET equation), surface film on liquid, catalytic activity at surfaces.

Adsorption from solution, Gibbs adsorption equation and its use in estimation of surface area of molecule, Electro-kinetic phenomenon. Zeta potential : its determination and significance, DLVO theory of colloid stability.

(B) Micelles:

Surface active agents, classification of surface active agents. Solubility of surfactants, micellization, hydrophobic interaction, critical micellar concentration (CMC) and its determination, factors affecting the CMC of surfactants, counter ion binding to micelles, thermodynamics of micellization - phase separation and mass action models, solubilization, microemulsion, reverse micelles. (Numericals)

UNIT-V : ELECTROCHEMISTRY: (15 Periods)

Debye-Huckel theory of interionic attraction (Qualitative account only) – relaxation effect and electrophoretic effect.

Activity, activity coefficient, mean activity coefficient, activity in electrolytic solutions - relation between concentration and activity, ionic strength, Debye-Huckel theory and dilute solutions (Debye-Huckel limiting law). Determination of activity coefficient - Dissociation constant of a monobasic acid by pH method polarization. Decomposition potential, over voltage concentration polarization. Influence of current density and temperature onover voltage, measurement of over voltage, Ionic discharge as the slow process at cathodes. afel and proton transfer theory of hydrogen over voltage. Electrified interface - electro-capillarity, electro-capillary maximum, Lippmann equation (surface excess). Numericals

UNIT-VI : (15 Periods)

(A) Molecular Spectroscopy:

Rotational spectra of diatomic molecule, selection rule, internuclear distance, intensity of spectral lines, effect of isotopic substitution, vibration spectra of diatomic molecule - Harmonic vibration, potential energy, selection rule, force constant, amplitude of vibration, Anharmonic vibration, Morse potential energy, Vibrational - Rotational - spectra. Harmonic and Nonharmonic. (Numericals)

(B) Nuclear Chemistry:

Radiation detectors - Gas ionization detectors - Principle, Ion chamber - Proportional counter, G M counter - Scintillation detector - Principle, features, Inorganic and organic scintillators, Solid state detectors, Radiochemical principle and use of tracers - Reaction - mechanism - structure determination, Surface area of a powder, Radiometric titration, Isotope dilution analysis. Neutron activation analysis.

Books Recommended:

1. Mathematics for Chemistry, Doggett and Sucliffe, Longman.
2. Mathematical preparation for Physical Chemistry, F. Daniels, McGraw Hill.
3. Quantitative Analysis, 6^{th} Ed., R. A. Day and A. L. Underwood, Prentice-Hall of India, 1993.
4. Experimental Physical Chemistry : A Laboratory Textbook, A. M. Halpernand J. H. Reeves Scott, Foresman and Co., 1988.
5. Physical Chemistry, P. W. Atkins, ELBS..
6. Chemical Kinetics, Ira N. Levine, Prentice Hall.
7. Kinetics and Mechanism of Chemical Transformations, J. Rajaraman and J. Kuriacose, McMillan.
8. Thermodynamics of Chemist, Glasstone, Van Nostrand Co.
9. Thermodynamic Properties of Non-electrolyte Solutions by W. E. Acree, Academic Press, 1984.
10. An Introduction to Chemical Thermodynamics, R. P. Rastogi and R. R. Misra, Vikas Publishing House, New Delhi.
11. Essentials of Nuclear Chemistry by H. J. Arnikar (Wiley Eastern Ltd., 1981).
12. Introduction to Polymer Science, V. R. Gowarikar, N. V. Vishwanathan and J. Sridhar, Wiley Eastern.
13. Text-book of Polymer Science by Billmeyer Wiley.
14. Quantum Chemistry Including Spectroscopy by B. K. Sen.
15. A Text-book of Physical Chemistry, Vol. 4, K. L. Kapoor McMillan, 1985.
16. Introduction to Molecular Spectroscopy, G. M. Barrow, McGraw-Hill.
17. Modern Spectroscopy, J. M. Hollas, John Wiley.
18. Basic Principles of Spectroscopy, R. Chang, McGraw-Hill.
19. Introduction to Physical Chemistry by A. M. Lesk, Prentice-Hall Inc., 1982.
20. Micelles, Theoretical and Applied Aspects, V. Morol, Plenum.
21. Introduction to Colloid and Surface Chemistry by Shaw.
22. Physical Chemistry by Protuonand Marron.
23. Statistical Thermodynamics by Gupta M. C.
24. Modern Electrochemistry, Vol. 1 & 2, J.O.M. Bookris and A.K.N. Reddy.
25. Introduction to Electrochemistry by Glasstone.

VEER NARMAD SOUTH GUJARAT UNIVERSITY

SYLLABUS FOR M.Sc. PART-I (PHYSICAL) CHEMISTRY
TO COME IN FORCE FROM JUNE-2002
PAPER-IV (PHYSICAL)

Max. Marks: 75 (External-52 + Internal-23) Total Periods: 90

UNIT-I : LIQUID STATE: (15 Periods)

The gal-like approach to liquids, the solid-like approach to liquids, some thermodynamic relations, internal pressure and its significance in liquids, equation of state, critical constants, intermolecular forces in liquids partition function and the use of statistical mechanics, the general nature of intermolecular forces in liquid. The attractive energy, polar and non-polar molecules, the electrostatic attraction energy, the induction energy, the London or dispersion energy, the resultant attractive energy, the repulsive energy, specific forces, potential functions for liquids, 12-6 potential, additivity of pair potential approximation, A classical partition function for liquids, correspondence principle, configurat-ional integral, configuration properties.

UNIT-II :
(A) GASEOUS STATE: (6 Periods)

Berthelot equation, Dietrice equation, Redlich-Kweng Equation, Virial Equation, Brigham-Bittice-Kammerling Onnes equations. Kinetic theory of gas viscosities, Calculation of collision diameter, Collision frequencies, mean free path and viscosity coefficients.

(B) SOLID STATE: (9 Periods)

Perfect and Imperfect Crystals, intrinsic and extrinsic defects, point defects, line and plane defects, vacancies, Schottky and Frenkel defects, colour centres, non-stoichiometry and defects, Metals insulators and semiconductors, electronic structure of solids, elementary idea about band theory, band structure of metals, insulators and semiconductures, intrinsic and extrinsic semiconductors.

UNIT-III : LIQUID CRYSTALS: (15 Periods)

Mesomorphic behaviour, Types of liquid crystals, thermotropic liquid crystals, lyotropic liquid crystals, positional order, bond orientational order, smectic liquid crystals, nematic liquid crystals, cholesteric liquid crystals, mesomorphism formed by amphiphilic compounds (lyotropic mesomorphism), effects of substituents, Re-entrant nematic phase, Disc like mesogens, Plastic crystal (cubic mesophase), liquid crystal polymers, liquid crystals in biological systems, Applications of liquid crystals, optical properties of liquid crystals.

UNIT-IV : SURFACE CHEMISTRY: (15 Periods)

Thermodynamic treatment of adsorption. Change in enthalpy, entropy and free energy of adsorptions, Insoluble monolayers, Langmuir film balance, Detailsof instrument and its working, Orientation of molecules in films and phase changes from pressure area curve, transfer of spread monolayers, LB films, Applications of adsorption from solution. Electrical Double layer – Gouy – Chapman & Stern theory.

UNIT-V : ELECTROCHEMISTRY: (15 Periods)

Principle of voltammetry, Dropping mercury electrode and its advantage, Residual current migration current, diffusion current, Ilkovic equation, Polarographic maxima and its suppression, Half wave potential. Factors affecting diffusion current, Derivation of cathodic polarographic wave equation and its interpretation, Interference of oxygen. Quantitative determination of unknown metal ions.

Ionic atmosphere, its thickness, Debye-Huckel-Onsagar equation, its validity in aqueous solution, Debye-Falkenhager effect, Wien effect.

UNIT-VI : (15 Periods)

(A) Nuclear Chemistry:

Nuclear Reactions - Conservation laws, energetics of nuclear raactions, Threshold energy, Reaction cross-section, Compound nucleus mechanism for nuclear reactions. Types of nuclear reaction, Nuclear Fission as a source of energy, nuclear chain reaction, condition for controlled chain reactions, principle nuclear reactors and type of reactors, Thermal nuclear reaction, Breeder reactor, Energy from nuclear fusion, Thermo nuclear reactions. Stellar energy, Thermo nuclear reaction on earth. Biological effect of radiation, effect of radiation on body, units of radiation energy.

(B) Kinetics:

General features of fast reaction, Study of fast reactions.

(i) Stopped flow method, (ii) Relaxation method, (iii) Flash photolysis, (iv) Molecular beam method.

Books Recommended:

1. Liquid and their properties by Temperley and Trevana.
2. An introduction to Liquid State, P. A. Egelstaff, Academic Press..
3. Introduction to Statistical Thermodynamics, T. L. Hill, Addison Wiley..
4. Molecular thermodynamics of fluid phase equilibria, J.M. Prausnitz, R. N. Lichten-thaler and E. G. Azevedo, Prentice-Hall, Inc, Englewood Cliffs, N.J., 1986.
5. Physical Chemistry by Berry, Rice and Ross.
6. Physical Chemistry by R. P. Varma.
7. Principle of the Solid State by H. V. Keer.
8. Solid State Chemistry by N. B. Hannuy.
9. Solid State Chemistry by L. Smart and Elaine Moore.
10. Thermotropic Liquid Crystals by G. W. Gray, John Wiley.
11. Solid State Chemistry and its applications, A. R. West, Plenum.
12. Thermodynamics for Chemists, Glasstone.
13. An Introduction to Electrochemistry by S. C. Lantone.
14. Modern Electrochemistry Vol. I & II, J. O. M. Bockris and A. K. N. Reddy, Plenum.
15. Essentials of Nuclear Chemistry by Arniker H. J. (Wiley Eastern Ltd., 1981).
16. Introduction to Nuclear Science, M. N. Sastri, East-West Press Pvt. Ltd., 1984.

VEER NARMAD SOUTH GUJARAT UNIVERSITY

SYLLABUS FOR M.Sc. PART-I CHEMISTRY
TO COME IN FORCE FROM JUNE-2002
PAPER-IV (ANALYTICAL)

Max. Marks: 75 (External-54 + Internal-21) Total Periods: 90

UNIT-I : QUANTITATIVE ANALYSIS: (15 Periods)

(1) Steps of Analysis and Computations:

Role of analytical chemistry, Classification of analytical methods. Classical and instrumental, Types of instrumental analysis, Selecting an analytical method. Neatness and cleanliness. Selecting and handling of reagents. Safety in analytical laboratory.

Steps of chemical analysis: Planning, sampling drying, preparation of solution, Removal of interference, Methods of computations, Calculations in titrimetry and gravimetry, calculations of direct and back titrations using molarity and normality (Numericals).

(2) Organic Analysis:

Micro and semi-micro determination of carbon, hydrogen, nitrogen using elemental analysers (any one), Use of Schoniger's flask combustion method for semi-micro determination of halogen and sulfur.

Determination of functional groups -

(i) Carbonyl group by oxime formation method
(ii) Polyhydric alcohols
(iii) Esters
(iv) Nitro groups
(v) Amino group
(vi) Azo group

(Numerical)

UNIT-II : ORGANIC REAGENTS AND NON-AQUEOUS TITRATIONS:

(15 Periods)

(1) Use of Organic Reagents in Analytical Chemistry:

Use of Acetyl acetone, Dithiozone, Neo-cuproin, 8-hydroxy quinoline, 1,10-phenanthroline, Dimethyl glyoxime in the spectrophoto-metric determination of metal ions and in selective extraction of metal ions.

(2) Non-Aqueous Titrations:

Levelling effect and differentiating ability of solvents, need for non-aqueous titrations, criteria to be considered in selecting solvents, Acidic and basic titrants and their standardisation, Indicating systems - Karl-Fischer titrations - Applications - Numericals.

UNIT-III : UV-VISIBLE SPECTROSCOPY: (15 Periods)

Interaction of radiation matter - Photometric accuracy - Simultaneous determinations of two components in a mixture - pK_{In} of indicator - Photometric titrations, Determination of metal to ligand ratio, analysis of drugs by UV-VIS spectrophotometry.

Review of components of UV-visible spectrophotometer - Source - Monochromator (prism and grating) - Sample handling detectors (photo-tube, PM tube and Diode array detectors) - Single beam and double beam instruments - Working of Spectronic-20 Backman DU-2 Spectrophotometer.

Fluorescence, Phosphorescence, Turbidimetry - Naphelometry principles and applications.

Quantitative analysis - Numericals.

UNIT-IV : DC-POLAROGRAPHY: (15 Periods)

Current voltage curves - Residual current, Kinetic current, Diffusion current, Migration current - Electrocapillary maxima - Maxima suppressors - Interference of oxygen.

Derivation of equation of cathodic and anodic waves - Tests of reversibility.

Half wave potential - Its determination and importance.

Effect of complexation on half wave potential - Determination of stability constants of complexes polarographically - Derivation of necessary equation.

Advantages and limitations of DME - Polarography with 2 and 3 electrodes - Polarography of organic compounds and its importance.

Ilkovic equation and terms involved - Quantitative analysis - Numericals.

Applications of DC polarography and its limitations.

UNIT-V : (15 Periods)

(1) Analytical methods based on electrolysis:

Electrolysis - Electrogravimetry - Factors affecting the quality of deposits - Applications.

Principle of coulometry - Controlled potential coulometry - Coulometric titrations (primary and secondary) applications - Acid-base titrations, Determination of arsenite, Mercaptants, Phenol.

(2) Amperometric titrations:

Principle of titrations - Titrations using DME & RPE - Nature of curves for different types of titrations - Biamperometric titrations - Karl-Fischer titration end point. Chronopotentiometry: Principle, apparatus and cell, applications.

(3) Statistical treatment of data:

Student's t-confidence limit - Testing for significance - Comparison of two means, two precisions - Criteria for rejection of an observation - The Q test - The control chart - Methods of least square - Numerical.

UNIT-VI : SOLVENT EXTRACTIONS: (15 Periods)

Review of distribution law - Distribution coefficient - Distribution ratio - Equations for the solute dissociating or associating in one phase - Successive extractions.

Extraction of metal ion with chelating agent with necessary equation - Multiple extractions - Craig pseudo counter current extractions - Apparatus for Craig extractions - Continuous counter current extractions - Extraction involving association of ion pairs - Elementary idea of extraction with crown ethers - Cryptans, Numericals.

Reference Books:

1. "Quantitative Analysis" by Day & Underwood (Prentice Hall of India), 6th edition.
2. "Analytical Chemistry" by Larry G. Hargis (Prentice-Hall International editions).
3. "Modern Methods of Analysis" by Packshok, Shields & Cains (Wiley International).
4. "Electroanalytical Chemistry" by Lingane.
5. "Vogel's text-book of Inorganic Quantitative Analysis" (5th edition), Longmann.
6. "Quantitative Chemistry by Brown-Bailey" (Prentice-Hall).
7. "Fundamentals of Analytical Chemistry" by Skoog & West (Holt-Rinchard & Winston, Inc.).
8. "Instrumental Methods of Chemical Analysis" by Ewing (McGraw-Hill).
9. "Instrumental Methods of Analysis" by Willard, Merritt & Dean (Van Nostrand Reinhold Co.), 6th edition.
10. "instrumental Methods of Analysis" by B. K. Sharma, Goel Publishing House, Meerut.
11. "Basic Concepts of Analytical Chemistry" (2nd edition) by Prof. S. M. Khopkar, New Age International (P) Ltd., Mumbai.