S. V. K. P. & Dr. K. S. RAJU ARTS & SCIENCE COLLEGE (A)

FIRST SEMESTER M.Sc. ORGANIC CHEMISTRY SYLLABUS

(With effect from 2023-24 Admitted batch)

(23OCHT11) Paper-I: GENERAL CHEMISTRY – I

UNIT-I

Basic Quantum Chemistry-I: Wave equation - interpretation of wave function-properties of wave function - Normalization and Orthogonalisation, Postulates of quantum mechanics; Operators - linear, non-linear and commutators of operators – Eigen functions and eigen values - Hermitian operator- Eigen values and Eigen functions of Hermitian operator; Unitary operator - setting up of operators to observables; position, linear momentum, energy and angular momentum – Eigen values of angular momentum operator.

UNIT-II

Basic Quantum Chemistry-II: Wave mechanics of simple systems with constant potential energy, particle in one- dimensional box, wave equation, quantized energies, zero point energy, normalized wave function, characteristics of wave function - factors influencing color - transition dipole moment integral - Symmetry arguments in deriving the selection rules - the concept of tunneling - particle in three-dimensional box, calculations using wave functions of the particle in a box- Wave mechanics of Rigid rotor, Hamiltonian operator - Wave mechanics of rigid rotator.

UNIT-III

Basic Quantum Chemistry-III: Wave mechanics of systems with variable potential energy - simple harmonic oscillator - solution of wave equation - characteristics of wave function - derivation of selection rules for simple harmonic oscillator - Hydrogen atom - Construction of Hamiltonian operator - Separation of variables in Schrodinger wave equation - solution of R(r), Φ (ϕ) and Θ (θ) equations. Probability density in 1S atomic orbital - shapes of orbitals.

UNIT-IV

Molecular Spectroscopy-I: Microwave and IR- Spectroscopy- Rotational spectra of diatomic molecules- Rigid rotor-Selection rules- Calculations of bond length- Isotopic effect in rotational spectra - Second order stark effect and its applications. Infrared spectra of diatomic molecules - harmonic and anharmonic oscillators - Selection rules - Calculation of force constant, anharmonicity constant and zero point energy - Overtones- Combination bands - Fermi resonance - simultaneous vibrational-rotational spectra of diatomic molecules.

UNIT- V

Molecular Spectroscopy-II: Raman and Electronic Spectra - Classical and quantum mechanical explanations - Rotational Raman spectra - Vibrational Raman spectra - Rotational fine structure of Raman spectra of diatomic molecules - Electronic spectra of diatomic molecules - Types of electronic transitions - Born Oppenheimer approximation - Vibrational Coarse structure - intensities of spectral lines - Franck-Condon principle - applications, Rotational Fine structure - band origin, band head and band shading.

References/ Text books

1. Fundamentals of Molecular spectroscopy: by C. N. Banwell
2. Molecular spectroscopy: by B. K. Sharma
3. Molecular spectroscopy: by Aruldas
4. Introductory quantum mechanics: by A. K. Chandra
5. Quantum chemistry: by R. K. Prasad

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FIRST SEMESTER M.Sc. ORGANIC CHEMISTRY SYLLABUS

(With effect from 2023-24 Admitted batch)

(23OCHT12) Paper- II: INORGANIC CHEMISTRY-I

UNIT- I

Structure & Bonding: Applications of VSEPR, Valence Bond and Molecular orbital theories in explaining the structures of simple molecules- role of p and d orbitals in π-bonding. Application of MO theory to Tetrahedral $[CoCl_4]^{2-}$, Square planar ($[PtCl_4]^{2-}$) and Octahedral complexes ($[CoF_6]^{3-}$, $[Co(NH_3)_6]^{3+}$). Classification of ligands based on π-bonding using MO theory.

UNIT-II

Inorganic cage and ring compounds – preparation, structure and reactions of boranes, carboranes, metallocarboranes. Electron counting in boranes – Wades rules (Polyhedral skeletal electron pair theory).

Heterocyclic inorganic ring systems: Boron–Nitrogen ($H_3B_3N_3H_3$), Phosphorus–Nitrogen ($N_3P_3Cl_6$) and Sulphur-Nitrogen (S_4N_4, $(SN)_x$) cyclic compounds.

UNIT-III

Coordination compounds: Crystal field theory - crystal field splitting patterns in octahedral, tetrahedral, tetragonal, square planar, square pyramidal and trigonal bipyramidal geometries. Calculation of crystal field stabilization energies. Factors affecting crystal field splitting energies – Spectrochemical series – Jahn – Teller effect, nephelauxetic effect – ligand field theory.

UNIT- IV

Term symbols – Russell – Sanders coupling – Hund's Rules – Hole Formalism, derivation of term symbols for p^1 –p^6 and d^1 – d^9 configurations of p and d orbitals. Spectroscopic ground states.

Magnetic properties of transition and inner transition metal complexes – spin and orbital moments –spin-orbit coupling and magnetic moments - Quenching of orbital momentum by crystal fields in complexes.

UNIT- V

Electronic spectra of transition metal complexes: Types of electronic transitions – d-d transitions - Selection rules, break down of selection rules – Orgel and Tanabe-Sugano diagrams for d^1 –d^9 octahedral and tetrahedral transition metal complexes of 3d series – Calculation of Dq, B and β parameters. Charge transfer spectra.

Reference books& Text books:

1. Advanced Inorganic Chemistry by F.A. Cotton and G. Wilkinson, IV Edition, John Wiley and Sons, New York, 1980.
2. Inorganic Chemistry by J.E. Huheey, III Edition, Harper International Edition, 1983.
3. Theoretical Inorganic Chemistry, II Edition by M.C. Day and J. Selbin, Affiliated East-West press pvt. Ltd., New Delhi.
4. Inorganic Chemistry by Shriver and Atkins, Oxford University Press (1999).
5. Inorganic Chemistry 5th Edition by Gary L. Miessler et al, Pearson Publications.

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FIRST SEMESTER M.Sc. ORGANIC CHEMISTRY SYLLABUS

(With effect from 2023-24 Admitted batch)

(23OCHT13) Paper –III: ORGANIC CHEMISTRY -I

UNIT – I

Nature of bonding in organic molecules and Aromaticity 15 Hrs

(A) *Electronic Effects and Reactive intermediates:*-Inductive effect, Mesomeric effect (Resonance), Hyperconjugation, Steric effect, Tautomerism, Generation, structure, stability and reactivity of carbocations, carbanions, free radicals, carbenes, nitrenes and arynes

(B) *Criteria of Aromaticity:*- Concept of Aromaticity, Huckle`s rule, aromaticity in benzenoid non-benzenoid compounds, Aromaticity in Fused-Ring Systems, Hetero-aromatic Systems, anti-aromaticity and homo-aromaticity and Pseudo aromaticity. *Annulenes:* Cyclobutadiene, Benzene,1,3,5,7-Cyclooctatetraene, [10] Annulenes, [12], [14], [16] and [18] annulenes,

UNIT – II

Stereo Chemistry &Molecular representation of organic molecules 12 Hrs

Molecular Symmetry and Chirality: Symmetry elements: Plane of Symmetry, Axis of Symmetry and Centre of Symmetry Definition and classification of Stereoisomers, Enantiomer, Diastereomer, Invertomers, Homomers, Epimers, Anomers, Configuration and Conformation Configurational nomenclature: D,L and R, S nomenclature, Molecules with a single chiral center, Molecules with two chiral centers; constitutionally unsymmetrical and symmetrical molecules.

UNIT – III 12 Hrs

(A) Geometrical Isomerism and Conformations of Cyclic Systems:- Cis-trans, E, Z- and Syn & anti nomenclature, Methods of determining configuration of Geometrical isomers using physical, spectral and chemical methods, Stability, Cis-trans inter conversion.Conformations of cyclobutane, cyclopentane, cyclohexane, mono and disubstitutedcyclohaxanes.

(B)Stereoisomerism in molecules without chiral Center -Axial chirality Allenes, Alkylidene cycloalkanes, spiranes, nomenclature. *Atropisomerism:* Biphenyl derivatives, nomenclature.

UNIT – IV

Heterocyclic compounds: 11 Hrs

Importance of heterocyclic compounds as drugs. Nomenclature of heterocyclic systems based on ring size,number and nature of hetero atoms. Chemistry of heterocyclic compounds, synthesis and reactivity of the following systems: Quinoline, Isoquinoline, Indole, Pyrazole, Imidazole, Oxazole, Isoxazole, Pyridazine, pyrimidine and Pyrazine.

UNIT - V

Chemistry of some typical natural products (Alkaloids and Terpenoids) 10 Hrs

A study of the following compounds involving their isolation, structure elucidation, synthesis and biogenesis of

Alkaloids; Atropine, Nicotine, and Quinine.

*Terpenoids:*α- Terpeneol, α-Pinene and Camphor.

Books Suggested:

1. Advanced Organic Chemistry-Reactions, Mechanism and structure, Jerry March, 6th Ed. (John Wiley & Sons).
2. Organic Chemistry, Paula YurkanisBruice, 4th Ed. (Printice Hall)
3. Organic chemistry-Clayden J. (Oxford)
4. Organic Chemsitry, Wade, L.G. Jr. 5th Ed. (Pearson)
5. Advanced Organic Chemistry: Reactions and mechanisms, Miller Bernard & Other, 2nd Ed. (Pearson)
6. Mechanism and Theory in Organic Chemistry, Thomas H. Lowry, Kathleen S. Richardson, Harper & Row, (Publishers, Inc.).
7. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, 6th Ed., (Longman).
8. Reaction Mechanism in Organic Chemistry, P.S. Kalsi, 2nd Ed. (New Age International).
9. Organic Chemistry, R. T. Morrison and R. N. Boyd (Prentice-Hall)
10. Stereochemistry to Organic Compounds, E.L. Eliel (John Wiley).
11. Stereochemistry, P.S. Kalsi, 5th Ed. (New Age International).
12. Organic Chemistry Structure and Reactivity, EgeSeyhan, 3rd Ed. (AITBS)
13. Heterocyclic Chemistry, J.A.Joule, K. Kills and G. F. Smith, Chapman and Hall
14. Heterocyclic Chemistry, T.L.Gilchrist, Longman Scientific Technical
15. Heterocyclic Chemistry, Raj.K. Bansal.
16. An Introduction to the Heterocyclic Compounds, R. M. Acheson, John Wiley.

REFERENCE BOOKS:

1. Chemistry of Natural Products, K.W.Bentley
2. Stereochemistry of carbon compounds by E.Eliel, John Wiley & Sons, Inc.
3. Stereochemistry to Organic Compounds, D. Nasipuri, 2nd Ed. (New Age International).
4. Chemistry of Natural products by R.S. KalsiKalyani Publishers. 1983.

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FIRST SEMESTER M.Sc. ORGANIC CHEMISTRY SYLLABUS

(With effect from 2023-24 Admitted batch)

(23OCHT14) Paper – IV: PHYSICAL CHEMISTRY-I

UNIT-I

Thermodynamics-I: Concepts of partial molar properties – partial molar volume and its significance; Determination of partial molar volume: Graphical method, intercept method and apparent molar volume method. Partial molar free energy, chemical potential, Variation of chemical potential with T and P. Gibbs-Duhem equation-derivation and significance. Phase equilibrium - Derivation of phase rule from the concept of chemical potential. *Ideal solutions* - Thermodynamics of mixing of liquids (ΔG_{mix}, ΔH_{mix}, ΔS_{mix}) - Thermodynamic properties of ideal solutions - Raoult's law; Thermodynamic properties of ideally dilute solutions - Henry's law. *Non ideal solutions*: Activities and activity coefficients; Standard state conventions for non ideal solutions - Determination of activity coefficients from vapour pressure measurements. Activity coefficients of non-volatile solutes using Gibbs-Duhem equation - Chemical equilibrium- effect of temperature on equilibrium constant - Van't-Hoff equation.

UNIT-II

Micelles and Macro molecules: Surface active agents, classification of surface active agents, micellization, hydrophobic interaction, Critical micellar concentration (CMC), factors affecting the CMC of surfactants, thermodynamics of micellization - phase separation and mass action models, Micellar solubilization, micro emulsion, reverse micelles.

Polymer- definition, types of polymers, electrically conducting, fire resistant, liquid crystal polymers, kinetics of free radical polymerization. Molecular mass- Number and mass average molecular weight, molecular weight determination- Osmometry, viscometry, ultracentrifugation and light scattering methods.

UNIT-III

Chemical Kinetics: Theories of reaction rates- Collision theory- Limitations, Transition state theory, Thermodynamic formulation of transition state theory. Effect of ionic strength on rates of reactions - Debye Huckel theory - Primary and secondary salt effects; Effect of dielectric constant on rates of reactions, Effect of substituent - Linear free energy relationships - Hammett equation-limitations, Taft equation; Kinetics of Consecutive reactions, parallel reactions, opposing reactions (Uni molecular steps only, no derivation).

UNIT-IV

Specific and general acid-base catalysis; Skrabal diagram; Steady state approximation - Protolytic and Prototropic mechanism - Enzyme catalysis- Michaelis -Menten mechanism. Derivation of Kinetic equation and Kinetic parameters. Lock and Key hypothesis - pH dependence of enzyme catalyzed reactions. Fast reactions, different methods of studying fast reactions- Flow methods: Continuous flow method and Stopped flow method - Relaxation methods: Shock tube method, temperature jump and pressure jump methods.

UNIT-V

Photochemistry: Electronic transitions in molecules, Franck-Condon principle. Electronically excited molecules - singlet and triplet states, spin-orbit interaction. Quantum yield and its determination; Actinometry - ferrioxalate and uranyl oxalate actinometers. Derivation of fluorescence and phosphorescence quantum yields. Quenching effect- Stern-Volmer equation. Photochemical equilibrium - Delayed fluorescence: E-type and P-type delayed fluorescence. Photochemical primary processes, types of photochemical reactions - Photodissocoation, Photoaddition and Photoisomerisation reactions with examples.

Books:

1. Physical Chemistry by Peter Atkins and Julio de Paula, Oxford UniversityPress.
2. Physical Chemistry by G.W. Castellon, Narosha PublishingHouse
3. Physical Chemistry by W.J.Moore, PrenticeHall
4. Thermodynamics for Chemists, SamuelGlasstone
5. Chemical Kinetics by K.J.Laidler, McGraw HillPub.
6. Photochemistry, R.P. Kundall and A. Gilbert, ThomsonNelson.
7. Polymer Chemistry byBillmayer
8. Introduction to Polymer Science, V.R. Gowriker, N.V.Viswanadhan and J. Sreedhar., WileyEaster.
9. Micells, Theoretical and applied aspects, V.Morol, Plenumpublishers.

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SECOND SEMESTER M.Sc. ORGANIC CHEMISTRY SYLLABUS

(With effect from 2023-24 Admitted batch)

(23OCHT21) Paper- I: GENERAL CHEMISTRY-II

UNIT-I

Approximation methods- Perturbation theory - Time independent perturbation theory (only first order perturbation is to be dealt with) - application to ground state energy of Helium atom - Variation principle – applications - calculation of zero-point energy of hydrogen atom and harmonic oscillator - many electron atom, Hamiltonian operator - Hartee's self-consistent field method - Hartee-Fock self-consistent field method.

UNIT-II

Bonding in molecules: Valence-Bond (VB) method application to H_2 molecule – Molecular Orbital theory - LCAO Approximation - Construction of trail function by the method of linear combinations. Variation parameters, secular equations and secular determinant - Application of MO theory to H_2^+ ion, The variation integral for H_2^+ ion, calculation of wave functions and energies for the bonding and anti-bonding MOs, Physical picture of bonding and anti-bonding wave functions, Energy diagram. Application of MO theory to H_2 molecule - Directed valence - Quantum mechanical concepts of SP^3, SP^2 and SP hybridisation.

UNIT-III

Molecular symmetry and Group Theory in Chemistry-I: Basic concepts of symmetry and Group theory - Symmetry elements, symmetry operations - Matrix representations for symmetry operations - point groups- Schoenflies symbols - Classification of molecules into point groups – Identification of point groups of molecules, linear, planar and three dimensional molecules - Axioms of Group theory - Group multiplication tables for C_{2v} and C_{3v} point groups -

UNIT-IV

Molecular symmetry and Group Theory in Chemistry-II: Similarity transformations and classes – Representations: reducible and irreducible representations, Mullikan symbols, Orthogonality theorem and its consequence – Properties of irreducible representations - Character table and its anatomy (need not to derive Character table) - Application of group theory to IR, Raman spectroscopy and transition metal complexes.

UNIT-V

Treatment of analytical data: Accuracy and precision - Classification of errors - Determination of Indeterminate errors - Minimization of errors - Absolute and Relative errors, propagation of errors - Distribution of Indeterminate errors - Gaussian distribution - Measures of central tendency - Measures of precision - Standard deviation - Standard error of mean- student's t- test - Confidence interval of mean - Testing for significance - Comparison of two means - F-test - Criteria of rejection of an observation - Significant figures and computation rules.

References/ Text books:

1. Introductory Quantum chemistry: by A. K. Chandra
2. Group theory for Chemistry: by A. K. Bhattacharya
3. Introductory Group theory for chemists : by George Davidson
4. Vogel's text book of quantitative analysis by Vogel
5. Fundamentals of Analytical chemistry: by Skoog and West
6. Quantum Chemistry: by N. Levine.

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SECOND SEMESTER M.Sc. ORGANIC CHEMISTRY SYLLABUS

(With effect from 2023-24 Admitted batch)

(23OCHT22) Paper- II: INORGANIC CHEMISTRY-II

UNIT-I

Metal cluster compounds - definition – evidences for existence of M-M bonds - conditions favorable for formation of M-M bonds – preparation, structure and bonding of the following metal cluster compounds.

$Re_2Cl_8^{2-}$, $Mo_2Cl_8^{4-}$, $Re_2(RCOO)_4X_2$, $Mo_2(RCOO)_4(H_2O)_2$, $Cr_2(RCOO)_4(H_2O)_2$, $Cu_2(RCOO)_4(H_2O)_2$, $Cr_2Cl_9^{3-}$, $Mo_2Cl_9^{3-}$, $W_2Cl_9^{3-}$, Re_3Cl_9, $Re_3Cl_{12}^{3-}$, $Mo_6Cl_8^{4+}$, $Nb_6X_{12}^{2+}$ and $Ta_6X_{12}^{2+}$.

UNIT-II

Organometallic compounds - 16 and 18 electron rules. Isoelectronicrelationship - Synthesis, structure, bonding and reactions of carbon monoxide, dinitrogen and nitric oxide complexes.Isolobal relationship – H, Cl, CH_3, $Mn(CO)_5$; S, CH_2, $Fe(CO)_4$; P, CH, $Co(CO)_3$. Synthesis, structure, bonding and reactions of metallocenes with special reference to ferrocene. Catalysis by Organometallic compounds

UNIT-III

Metal Ligand equilibria in solution: Stepwise and overall formation constants and their interaction– trends in stepwise constants – factors affecting the stability of metal complexes– Pearson's theory of hard and soft acids and bases (HSAB), chelate effect and its thermodynamic origin, determination of stability constants of complexes–spectrophotometric method and pH–metric method.

UNIT- IV

Inorganic Reaction Mechanisms: Reactivity of metal complexes–inert and labile complexes.Explanation of lability on the basis of VBT & CFT. Substitution reactions of metal complexes – D, Id, Ia and A mechanisms – Ligand replacement reactions of octahedral complexes – Acid hydrolysis – factors affecting acid hydrolysis – Anation and Base hydrolysis of Cobalt(III) complexes. Ligand displacement reactions of square planar complexes of platinum (II). Factors affecting square planar substitution – trans effect (theories).

UNIT- V

Bio-Inorganic Chemistry & Electron transfer reactions : Metalloporphyrins with special reference to Haemoglobin& Myoglobin. Biological role of alkali and alkaline earth metal ions with special reference to Ca^{2+}.Biological and abiological Nitrogen Fixation.

Electron transfer reactions of complexes – concept of complementary and non-complementary reactions with examples.Inner and outer sphere mechanisms.

Text books:

1. Advanced Inorganic Chemistry by F.A. Cotton and R.G. Wilkinson, IV Edition, John, John Wiley and Sons, New York, 1980.
2. Inorganic Chemistry by J.E. Huheey, III edition, Harper International Edition, 1983.
3. Organometallic Chemistry-A unified approach by A. Singh and R.C. Mehrotra, Wiley Eastern Ltd.
4. Inorganic Chemistry by Shriver and Atkins, Oxford University Press (1999)
5. Theoretical Inorganic Chemistry, II Edition by M.C. Day and J. Selbin, Affiliated East-West press Pvt. Ltd., New Delhi.
6. Mechanisms of Inorganic reactions in solution by D.Benson, MCgraw Hill, London, 1968.

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SECOND SEMESTER M.Sc. ORGANIC CHEMISTRY SYLLABUS

(With effect from 2023-24 Admitted batch)

(23OCHT23) Paper-III: ORGANIC CHEMISTRY-II

UNIT-I

Reaction Mechanism **10 Hrs**

Aliphatic Nucleophilic Substitution and Nucleophilic Aromatic substitution: Stereochemistry of S_N2 and S_N1 mechanisms, Neighboring Group Participation (Anchimeric assistance), NGP by O, S, N: Aromatic Nucleophilic substitution: SN2 (Ar) (Addition – Elimination), SN1(Ar) and benzyne mechanisms (Elimination - Addition); evidence for the structure of benzyne. Von Richter Sommelet-Hauser and Smiles rearrangements.

UNIT-II **10 Hrs**

Elimination Reactions:Type of elimination reactions, mechanisms, Stereochemistry and Orientation, Hofmann and Saytzeff rules, Syn elimination versus anti-elimination, competition between elimination and substitution, dehydration, dehydrogenation, dehalogenation, decarboxylative eliminations and pyrolytic eliminations

UNIT-III

Addition Reactions **15 Hrs**

(A) Addition to Carbon – Carbon Multiple Bonds:Mechanistic and stereo chemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, region and chemo selectivity, orientation and reactivity, Hydrogenation of double and triple bonds, hydrogenation of aromatic rings, Hydroboration.

(B) Addition to Carbon-Hetero Multiple Bonds: Steric course of addition reactions to C=O and C=N, Aldol, Cannizzaro, Perkin, Knoevenagel, Claisen-Schmidt, Claisen, Dieckman, Benzoin and Stobbe condensations, Reformatsky reaction, Tollen's reaction, Prins reaction: Wittig, Grignard, Mannich, and Michael reaction, Hydrolysis of Carbon-Nitrogen bond, Isocyanates and isothioyanates.

UNIT-IV

Molecular Rearrangements **12 Hrs**

Types of molecular rearrangements, migratory aptitude*;*

(A) Rearrangements to electron deficient carbon: Pinacol-pinacolone, Wagner-Meerwein, , Dienone – Phenol, Arndt-Eistert synthesis*;*

(B) Rearrangements to electron deficient nitrogen: Beckmann, Hofmann, Curtius, Schmidt and Lossen rearrangements.

(C) *Rearrangements to electron deficient oxygen:* Baeyer-villiger, Hydro peroxide rearrangement and Dakin rearrangements; Neber rearrangement, Benzil-Benzilic acid and Favorskii rearrangements

UNIT-V

Spectroscopy: Basic principles and importance of UV, IR, NMR and Mass. **13 Hrs**

(A) UV Spectroscopy: Introduction**,** Absorption Laws (Lambert's Law and Beer's Law), Chromophore, Auxo Chrome,

(B) IR Spectroscopy: Introduction, Finger Print Region

(C) NMR Spectroscopy: Introduction, Nuclear Spin, Nuclear Resonance, Shielding, Deshielding and Chemical Shift

(D) Mass Spectroscopy: Introduction, Fragmentation pattern of Aldehydes and Ketones.

Books Suggested:

1. Advanced Organic Chemistry-Reactions, Mechanism and structure, Jerry March, 6th Ed. (John Wiley & Sons).
2. Modern Organic Reactions, H. O. House (Benjamin)
3. Structure and Mechanism in Organic Chemistry, C.K. Inglod (Comell University Press).
4. Organic Chemistry, Paula YurkanisBruice, 4th Ed. (Printice Hall)
5. Organic Chemistry, Salmons, P.W. & Others, 8th Ed. (John Wiley & Sons)
6. Advanced Organic Chemistry: Reactions and mechanisms, Miller Bernard & Other, 2nd Ed. (Pearson)
7. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, 6th Ed., (Longman).
8. Reaction Mechanism in Organic Chemistry, P.S. Kalsi, 2nd Ed. (New Age International).
9. Stereochemistry to Organic Compounds, E.L. Eliel (John Wiley). 13. Stereochemistry to Organic Compounds, Nasipuri, 2nd Ed. (New Age International).
10. Stereochemistry, P.S. Kalsi, 5th Ed. (New Age International). Organic Chemistry Structure and Reactivity, Ege Seyhan, 3rd Ed. (AITBS)
11. Spectroscopic Methods in Organic Chemistry- Forth Edition, D.H. Williams and I. Fleming Tata - McGraw Hill, New Delhi, 1990.
12. Organic Spectroscopy- Second Edition, W. Kemp, ELBS Macmillan, 1987.
13. Applications of absorption spectroscopy of Organic Compounds J.R.Dyer,Prentice Hall of India, New Delhi, 1984.
14. Spectrometric identification of Organic Compounds-Fourth Edition, R.M. Silverstein: G.C.Vassiellr and T.C. Merill, Johne Willey, Singapore, 1981.

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SECOND SEMESTER M.Sc. ORGANIC CHEMISTRY SYLLABUS

(With effect from 2023-24 Admitted batch)

(23OCHT24) Paper – IV: PHYSICAL CHEMISTRY-II

UNIT-I

Physical methods of molecular structural elucidation: Magnetic susceptibility – Gouy balance method for measuring magnetic susceptibility - NMR: Principle and theory, Nature of spinning particle and its interaction with magnetic field - Chemical shift and its origin. Spin-Spin interaction, Application of NMR to structural elucidation: Structure of ethanol, dimethylformamide, styrene and acetophenone – NMR instrumentation.

UNIT-II

Electron Spin Resonance: Principle and theory - g-factor, presentation of ESR spectra, line shapes and line widths - hyperfine interactions, H atom, D atom and CH_3 radical – Reference used in ESR and determination of g-factor - Applications of ESR studies to the structure of free radicals and metal complexes - zero field splitting, Kramer's degeneracy – ESR instrumentation.

UNIT -III

Thermodynamics-II- Brief review on entropy; entropy changes accompanying specific process – expansion, phase transition, heating or cooling - Nernst heat theorem, limittions; Third law of thermodynamics - Determination of the absolute entropy of solids, liquids and gases - Apparent exceptions to Third law of thermodynamics.

Statistical Thermodynamics: Objectives of statistical thermodynamics, Concept of distributions, Types of ensembles. Thermodynamic probability, Most probable distribution, Maxwell-Boltzmann distribution Law – Partition Function, (Definition and significance): Molar and molecular partitions - translational, rotational, vibrational and electronic partition functions - Relation between thermodynamic functions (E, H, S, G and C_v) and the partition functions.

UNIT-IV

Electrochemistry I: Electrochemical cell- Galvanic and electrolytic cell. Concentration cell with and without transference, Effect of complexation on redox potential – ferricyanide / ferrocyanide couple, Iron (III) phenonthroline / Iron (II) phenonthroline couple. Determination of standard potential, activity coefficients and solubility product from EMF

data.

Bjerrum theory of ion association (elementary treatment) - Concept of activity and activity coefficients in electrolytic solutions. The mean ionic activity coefficient. Debye-Huckel theory of electrolytic solutions. Debye-Huckel limiting law (derivation not required), Calculation of mean ionic activity coefficient; Limitations of Debye-Huckel theory. Effect of dilution on equivalent conductance of electrolytes - Anomalous behavior of strong electrolytes. Debye Huckel-Onsagar equation – verification and limitations, Fuel Cells.

UNIT-V

Electrochemistry II: The electrode-electrolyte interface. The electric double layer. The Helmholtz-Perrin parallel-plate model, the Gouy-Chapman diffuse-charge model and the Stern model.

Electrodics: Charge transfer reactions at the electrode-electrolyte interface. Exchange current density and over-potential. Derivation of Butler-Volmer equation, High field approximation, Tafel equation, Low field equilibrium, Nernst equation. Voltametry - Concentration polarization, experimental techniques.

Books:

1. Text book of Physical Chemistry by Samuel Glasstone, McMillanPub.
2. Physical Chemistry by W.J.Moore, PrenticeHall
3. Physical Chemistry by G.W. Castellon, Narosha PublishingHouse
4. Physical Chemistry by Peter Atkins and Julio de Paula, Oxford UniversityPress.
5. Modern Electrochemistry, 2A & 2B, JOM Bockris&A.K.N.Reddy, Plenumpublishers
6. Introduction to Electrochemistry,S.Glasstone.
7. Fundamentals of Molecular Spectroscopy,Banwell
8. Spectroscopy by Straw &Walker.
9. Statistical thermodynamics ,M.C.Gupta
10. Statistical Thermodynamics,M.Dole
