



**MAHATMA GANDHI UNIVERSITY
NALGONDA**

**DEPARTMENT OF CHEMISTRY
M.Sc. CHEMISTRY SYLLUBUS
Effective from Academic Year 2023-24**

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Ruppa, Yoy, P. Reddy, M. Jyoti, K. Reddy, 22/11/2023, 22/11/2023



MAHATMA GANDHI UNIVERSITY, NALGONDA
DEPARTMENT OF CHEMISTRY
(Effective from the academic year 2023-2024)

SEMESTER –I

Paper-I: CH 101T (INORGANIC CHEMISTRY)

IC 01: Symmetry of Molecules

IC 02: Bonding in Metal Complexes - I

IC 03: Coordination Equilibria

IC 04: Ligational Aspects of Diatomic molecules

IC-01: Symmetry of Molecules:

15 Hrs

Symmetry Operations and Symmetry Elements: Rotational axis of symmetry and types of rotational axes, plane of symmetry and types of planes, improper rotational axis of symmetry, inversion center and identity element. Molecular Point Groups: Definition and notation of point groups, Classification of molecules based on molecular point groups. Systematic assignment of point groups to molecules (flow chart). Exercises in molecular point groups: C_1 , C_s , C_i , C_n , C_{nv} , C_{nh} , $C_{\infty v}$, D_n , D_{nh} , D_{nd} , $D_{\infty h}$, S_n (n =even), T_d (CH_4 , SiH_4), O_h (SF_6), I_h ($B_{12}H_{12}^{2-}$), K_h . Descent and ascent in symmetry with substitution (eg. NH_3 , CH_4 , PCl_5 , ML_6). Symmetry restrictions on dipole moment. Symmetry criteria for optical activity.

IC-02: Bonding in Metal Complexes – I:

15 Hrs

Crystal Field Theory: Salient features of CFT. d-orbital splitting patterns in regular octahedral, tetrahedral, square planar, tetragonally distorted octahedral, Jahn-Teller theorem, trigonal bipyramidal, trigonal planar, pentagonal bipyramidal, and linear geometries. Factors influencing magnitude of Δ_o . Concept of weak field and strong fields. Calculation of crystal field stabilization energies (CFSE's) in six and four coordinate complexes. Applications of CFSE-normal and inverse spinels.

Magnetic properties of transition metal complexes: Types of magnetic behavior. Magnetic susceptibility. Calculation of magnetic moment from magnetic susceptibility. Spin only formula. Quenching of orbital angular momentum. Determination of magnetic moment from Guoy's method. Applications of magnetic moment data for the determination of oxidation states, bond type and stereochemistry. Spin crossover.

IC-03: Coordination Equilibria:

15Hrs

Solvation of metal ions. Metal complex formation in solution. Binary metal complexes. Stability constants: Types (concentration, Thermodynamic and Conditional), stepwise and overall stability constants and relationships between them. Factors influencing the stability constants - (i) Metal ion effects: charge, size, charge/size IP, crystal field effect (Irving-William's order of stability), Jahn-Teller effect. (ii) Ligand effects: Basicity, substituent effect, steric, chelate (size and number of chelate rings), macrocyclic and cryptate effects (crown ethers, cryptands, size match selectivity or concept of hole size and its limitations), macrocycles with pendent groups.

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Pearson's theory of hard and soft acids and bases (HSAB): Principle and applications. Methods used for the determination of stability constants: pH metric, spectrophotometric and polarographic methods. Ternary metal complexes: Definition, formation of ternary metal complexes, step-wise and simultaneous equilibria with simple examples.

IC – 04: Ligational Aspects of Diatomic molecules:

15 Hrs

Metal Carbonyls:- Carbon monoxide as a ligand – Molecular orbitals of CO - Donor and Acceptor molecular orbitals of CO; Bonding modes of CO- Terminal and Bridging; Evidence for multiple bonding from Bond lengths and Stretching frequencies; 18 Valence electron rule and its application.

Metal Nitrosyls:- NO as a ligand – Molecular orbitals of NO – Donor and Acceptor components; Bonding modes of NO – Terminal (Linear, Bent) and Bridging; Structural aspects of $[\text{IrCl}(\text{PPh}_3)_2(\text{CO})(\text{NO})]^+$ and $[\text{RuCl}(\text{PPh}_3)_2(\text{NO})_2]^+$. Stereo chemical control of valence in $[\text{Co}(\text{diars})_2(\text{NO})]^{2+}$ and $[\text{Co}(\text{diars})_2(\text{NO})(\text{SCN})]^+$.

Metal Dinitrogen Complexes:- N_2 as a ligand – Molecular orbitals of N_2 ; Bonding modes – Terminal and Bridging; Stretching frequencies; Structures of Ru (II) and Mo (0) dinitrogen complexes; Chemical fixation of dinitrogen.

References:

1. Chemical applications of group theory, F Albert Cotton, 3rd Edition, Wiley India (2009).
2. Symmetry and Spectroscopy of Molecules, K.Veera Reddy, New Age Int. (P) Ltd. (2002)
3. Symmetry in Chemistry, Hans H Jaffe, Milton Archin, Dover publications Inc (2002)
4. Molecular symmetry and group theory, Allen Vincent, 2nd Edition, John Wiley & Sons Ltd. (2010)
5. Advanced Inorganic Chemistry, F.A.Cotton & G.Wilkinson, 3rd Edition, Wiley Interscience Publications (1972).
6. Advanced Inorganic Chemistry. F.A.Cotton, G.Wilkinson, C.A.Murillo & M.Bochmann, 6th Edition, Wiley Interscience Publications N.Y (1999).
7. Inorganic Chemistry, J.E. Huheey, K.A.Keiter and R.L.Keiter, 4th Edition, Harper Cottens College Publications (1993).
8. Inorganic Chemistry, Keith F.Purcell and John C.Kotz, Holt-Saunders Int. Edn.London (1977).
9. Principles of Inorganic Chemistry, Puri, Sharma, Kalia, 3rd Edition, Vishal Publications (2022).
10. Metal complexes in Aqueous Solutions, A.E Martell and Robert Hancock, Springer Science (1996).

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Paper-II: CH 102T (ORGANIC CHEMISTRY)

OC-01: Stereochemistry

OC-02: Reaction mechanism-I

OC-03: Carbohydrates and Proteins

OC-04: Heterocyclic compounds

OC-01: Stereochemistry

15Hrs

Molecular representations: Wedge, Fischer, Newman and Saw-horse formulae, their description and interconversions.

Molecular Symmetry & Chirality: Symmetry operations and symmetry elements (C_n & S_n). Criteria for Chirality. Desymmetrization.

Axial, planar and helical chirality: Configurational nomenclature: Axially chiral allenes, spiranes, alkylidene cycloalkanes, chiral biaryls, atropisomerism. Planar chiral ansa compounds and trans-cyclooctene. Helical chiral compounds

Relative and absolute configuration: Determination of absolute configuration by chemical correlation methods.

Racemisation, racemates and resolution techniques: Resolutions by direct crystallization, diastereoisomer salt formation chiral chromatography and asymmetric transformation.

Determination of configuration in E, Z-isomers: Spectral and Chemical methods of configuration determination of E, Z isomers. Determination of configuration in aldoximes and ketoximes.

OC-02: Reaction mechanism-I

15Hrs

Electrophilic addition to carbon carbon double bond: Stereoselective addition to carbon carbon double bond; *anti* addition- Bromination and epoxidation followed by ring opening. *Syn* addition of OsO_4 and $KMnO_4$.

Elimination reactions Elimination reactions E_2 , E_1 , E_1CB mechanisms. Orientation and stereo selectivity in E_2 eliminations. Pyrolytic *syn* elimination and α -elimination, elimination Vs substitution.

Determination of reaction mechanism: Determination of reaction mechanism: Energy profiles of addition and elimination reactions, transition states, product isolation and structure of intermediates, use of isotopes, chemical trapping, crossover experiments. Use of IR and NMR in the investigation of reaction mechanism.

OC-03: Carbohydrates and Proteins

15Hrs

Carbohydrates: Determination of the relative and absolute configuration in D (+) glucose and D (-) fructose. Proof for the chair conformation of D (+) glucose. Occurrence, importance and synthesis of monosaccharides containing functional groups such as amino, halo and sulphur. Structure elucidation and synthesis of sucrose. Conformational structures of D (+) ribose, 2-deoxyD-ribose, sucrose, lactose maltose and cellobiose. Structural features of starch, cellulose and chitin.

Proteins: Acid and enzymatic hydrolysis of proteins. Determination of the amino acid sequence in polypeptides by end group analysis. Chemical synthesis of di and tripeptides. Merrifield's solid phase synthesis.

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OC-4: Heterocyclic Compounds

15Hrs

Importance of heterocyclic compounds as drugs. Nomenclature of heterocyclic systems based on ring size, number and nature of hetero atoms. Synthesis and reactivity of indole, benzofuran, benzothiophene, quinoline, isoquinoline, coumarin, chromone, carbazole and acridine.

References:

1. Stereochemistry of carbon compounds by Ernest L Eliel and Samuel H. Wilen
2. Stereochemistry of organic compounds- Principles and Applications by D. Nasipuri
3. Heterocyclic Chemistry, T.L. Gilchrist, Longman UK Ltd, London (1985).
4. Benzofurans A. Mustafa, Wiley-Interscience, New York (1974).
5. Heterocyclic Chemistry, 3rd Edn J.A. Joule, K. Mills and G. F. Smith, Stanley Thornes Ltd, UK, (1998)
6. The Chemistry of Indole, R.J. Sunderberg, Academic Press, New York (1970).
7. An introduction to the chemistry of heterocyclic compounds, 2nd Edn. R. M. Acheson, Interscience Publishers, New York, 1967.
8. Advanced Organic Chemistry by Jerry March
9. Mechanism and Structure in Organic Chemistry S. Mukerjee
10. Guide Book to mechanism in Organic Chemistry, 6th Edition, Peter Sykes.
11. Organic Chemistry by Graham Solomous and Craig Fryhle.
12. Organic Chemistry by RT Morrison and RN Boyd.
13. Organic Chemistry, Vol. 2 by I. L. Finar.
14. Organic Chemistry: Structure and Reactivity by Seyhan Ege.

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Paper-III: CH 103 T (PHYSICAL CHEMISTRY)

PC-01: Thermodynamics-I

PC-02: Electrochemistry

PC-03: Quantum Chemistry-I

PC-04: Chemical Kinetics

PC-01: Thermodynamics-I

15 Hrs

Brief review of concepts of I and II laws of thermodynamics. Concept of entropy. Entropy as a state function. Calculation of entropy changes in various processes. Entropy changes in an ideal gas. Entropy changes on mixing of ideal gases. Entropy as a function of V and T.

Entropy as a function of P and T. Entropy change in isolated systems- Clausius inequality. Entropy change as criterion for spontaneity and equilibrium.

Third law of thermodynamics. Evaluation of absolute entropies from heat capacity data for solids, liquids and gases. Standard entropies and entropy changes of chemical reactions. Helmholtz and Gibbs free energies (A and G). A and G as a criterion for equilibrium and spontaneity. Physical significance of A and G. Driving force for chemical reactions- relative signs of ΔH and ΔS .

Thermodynamic relations. Gibbs equations. Maxwell relations. Temperature dependence of G. Gibbs- Helmholtz equation. Pressure dependence of G.

Chemical potential: Gibbs equations for non-equilibrium systems. Material equilibrium. Phase equilibrium. Clapeyron equation and Clausius-Clapeyron equation.

Conditions for equilibrium in a closed system. Chemical potential of ideal gases. Ideal-gas reaction equilibrium-derivation of equilibrium constant. Temperature dependence of equilibrium constant-the Van't Hoff equation.

PC-02: Electrochemistry

15 Hrs

Electrochemical Cells: Derivation of Nernst equation – problems. Chemical and concentration cells (with and without transference). Liquid junction potential – derivation of the expression for LJP – its determination and elimination. Applications of EMF measurements: Solubility product, potentiometric titrations, determination of transport numbers, equilibrium constant measurements. Decomposition potential and its significance. Electrode polarization – its causes and elimination. Concentration overpotential.

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. Extended Debye-Huckel law.

Theory of electrolytic conductance. Derivation of Debye-Huckel-Onsager equation – its validity and limitations.

Concept of ion association – Bjerrum theory of ion association (elementary treatment) -ion association constant – Debye-Huckel-Bjerrum equation.

PC-03: Quantum Chemistry-I

15 Hrs

Black body radiation-Planck's concept of quantization-Planck's equation, average energy of an oscillator (derivation not required). Wave particle duality and uncertain principle significance of these for microscopic entities. Emergence of quantum mechanics. Wave mechanics and Schrodinger wave equation. Operators-operator algebra. Commutation of operators, linear operators. Complex functions. Hermitian operators. Operators $\square\square$ and \square^2 . Eigenfunctions and eigenvalues. Degeneracy. Linear combination of eigenfunctions of an operator. Well behaved functions. Normalized and orthogonal functions.

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Postulates of quantum mechanics. Physical interpretation of wave function. Observables and operators. Measurability of operators. Average values of observables. The time dependent Schrodinger equation. Separation of variables and the time-independent Schrodinger equation.

Theorems of quantum mechanics. Real nature of the eigen values of a Hermitian operator significance. Orthogonal nature of the eigen values of a Hermitian operator-significance of orthogonality. Expansion of a function in terms of eigenvalues. Eigen functions of commuting operators-significance. Simultaneous measurement of properties and the uncertainty principle.

PC-04: Chemical Kinetics

15 Hrs

Theories of reaction rates: Collision theory, steric factor. Transition state theory. Reaction coordinate, activated complex and the transition state. Thermodynamic formulation of transition state theory. Activation parameters and their significance. The Eyring equation. Unimolecular reactions and Lindemann's theory.

Complex reactions- Opposing reactions, parallel reactions and consecutive reactions (all first order type). Chain reactions-general characteristics, steady state treatment. Example- H₂-Br₂ reaction. Derivation of rate law. Effect of structure on reactivity- Linear free energy relationships. Hammett and Taft equations-substituent (ρ and ρ^*) and reaction constant (ρ and ρ^*) with examples. Deviations from Hammett correlations. reasons- Change of mechanism, resonance interaction. Taft four parameter equation. Correlations for nucleophilic reactions. The Swain – Scott equation and the Edward equation. The reactivity-selectivity principle and the isoselectivity rule. The intrinsic barrier and Hammond's postulate.

References:

1. Atkin's Physical Chemistry, Peter Atkins and Julio de Paula, Oxford University press
2. Physical Chemistry, Ira N. Levine, McGraw Hill
3. Physical Chemistry-A Molecular approach, D.A. McQuarrie and J.D. Simon, Viva Books Pvt. Ltd
4. Molecular Thermodynamics, D.A. McQuarrie and J.D. Simon, University Science Books
5. Quantum Chemistry, Ira N. Levine, Prentice Hall
6. Introduction to Quantum Chemistry, A.K. Chandra, Tata McGraw Hill
7. Chemical Kinetics, K.J. Laidler, McGraw Hill
8. Kinetics and Mechanism of Chemical Transformations, J. Rajaraman and J. Kuriacose, McMillan
9. Introduction to Electrochemistry, S. Glasstone
10. Modern Electrochemistry, J. O. M. Bockris & A. K. N. Reddy, Plenum
11. Principles of physical chemistry, Samuel H. Maron and Carl F. Prutton, Oxford & IBH
12. The Physical Basis of Organic Chemistry by Howard Maskill, Oxford University Press (New York)
13. Chemical Kinetics and Reaction Mechanisms, J. H. Espenson, McGraw Hill
14. Physical Organic Chemistry, N. S. Isaacs, ELBS

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Paper-IV: CH 104 T (ANALYTICAL TECHNIQUES and SPECTROSCOPY- I)

ASP 01: Techniques of Chromatography

ASP 02: NMR spectroscopy-I (¹H NMR)

ASP 03: Rotational and Vibrational spectroscopy

ASP 04: Electronic spectroscopy

ASP-01: Techniques of Chromatography

15 Hrs

i. Introduction, Classification of chromatographic techniques, differential migration rates, partition ratio, retention time, relation between partition ratio and retention time, capacity factor, selectivity factor. Efficiency of separation- resolution, diffusion, plate theory, rate theory and problems.

ii. **GC:** Principle, instrumentation, detectors- TCD, FID, ECD. Derivatisation techniques, PTGC.

iii. **HPLC:** Principle, instrumentation, detectors- UV detectors, Photodiode array detector, fluorescence detector.

iv. Applications: Methods of quantitation for GC and HPLC: GC analysis of hydrocarbons in a mixture, GC assay of methyl testosterone in tablets, atropine in eye drops. HPLC assay of paracetamol and aspirin in tablets.

ASP 02: NMR Spectroscopy-I (¹H NMR)

15 Hrs

¹H NMR spectroscopy: Magnetic properties of nuclei, Principles of NMR. Instrumentation, CW and pulsed FT instrumentation, equivalent and non equivalent protons, enantiotopic and diastereotopic protons, Chemical shifts, factors affecting the chemical shifts, electronegativity and anisotropy, shielding and deshielding effects, Signal integration, Spin-spin coupling: vicinal, geminal and long range, Coupling constants and factors affecting coupling constants. Applications of ¹H NMR spectroscopy: Reaction mechanisms (cyclic bromonium ion, electrophilic and nucleophilic substitutions, carbocations and carbanions), E,Z isomers, conformation of cyclohexane and decalins, keto-enol tautomerism, hydrogen bonding, proton exchange processes (alcohols, amines and carboxylic acids), C-N rotation. Magnetic resonance imaging(MRI). ¹H NMR of organic molecules and metal complexes: ethyl acetate, 2- butanone, mesitylene, paracetamol, aspirin, ethylbenzoate, benzyl acetate, 2-chloro propionic acid, [HNi(OPe₃)₄]⁺, [HRh(CN)₅] Rh I=1/2, [Pt(acac)₂].

ASP 03 :Rotational and Vibrational spectroscopy

15 Hrs

a). Microwave Spectroscopy: Classification of molecules based on moment of inertia. Diatomic molecule as rigid rotator and its rotational energy levels. Selection rules (derivation not required). Calculation of bond lengths from rotational spectra of diatomic molecules. Isotope effect on rotational spectra. Calculation of atomic mass from rotational spectra. Brief description of microwave spectrometer.

b). Vibrational Spectroscopy. Vibrational energy levels of diatomic molecules, selection rules (derivation not required). Calculation force constant from vibrational frequency. Anharmonic nature of vibrations. Fundamental bands, overtones and hot bands, Fermi Resonance. Vibration-rotation spectra diatomic molecules. Vibrations of poly atomic molecules. Normal modes of vibration, concept of group frequencies. Characteristics of vibrational frequencies of functional groups; Stereochemical effects on the absorption pattern in carbonyl group, cis-trans isomerism and hydrogen bonding. Isotopic effect on group frequency. IR spectra of metal coordinated NO₃⁻, SO₄²⁻ and CO₃²⁻ ions.

Raman Spectroscopy- Quantum theory of Raman effect, Rotational Raman and Vibrational Raman spectra, Stokes and anti- Stokes lines. Complementary nature of IR and Raman spectra.

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ASP 04:Electronic spectroscopy

15 Hrs

Electronic spectroscopy: Electronic spectra: Elementary energy levels of molecules-selection rules for electronic spectra; types of electronic transitions in molecules. Chromophores: Conjugated dienes, trienes and polyenes, unsaturated carbonyl compounds, benzene and its derivatives, Woodward-Fieser rules. Polynuclear aromatic hydrocarbons and diketones. Solvent and structural influences on absorption maxima, stereochemical factors. Cis-trans isomers, and cross conjugation. Beer's law application to mixture analysis and dissociation constant of a weak acid.

References:

1. Fundamentals of Molecular Spectroscopy, Banwell and McCash.
2. Introduction to Molecular Spectroscopy, G.M. Barrow.
3. Absorption Spectroscopy of Organic Compounds, J.R. Dyer.
4. Biochemistry: Hames and Hooper.
5. Introduction to Spectroscopy, Pavia Lampman Kriz.
6. Pharmaceutical analysis, Watson
7. NMR in Chemistry- A multinuclear introduction, William Kemp.
8. Organic Spectroscopy, William Kemp. 10
9. Spectroscopy of organic compounds, P.S. Kalsi.
10. Structural methods n Inorganic chemistry, E.A.V Ebsworth.

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Paper CH 151P: Inorganic Chemistry Lab-I : 4 hrs/week

I. Preparation of Complexes

1. Hexaammine nickel (II) chloride
2. Tris (acetylacetonato) manganese(III)
3. Tris(ethylenediamine) nickel(II) thiosulphate

II. Calibrations

4. Calibration of weights
5. Calibration of pipettes
6. Calibration of standard flasks
7. Calibration of burette.

III. Titrimetric Analysis

8. Estimation of Fe^{+2} by cerimetry
9. Estimation of Ni^{+2} by complexometry (direct titration method)
10. Estimation of Cu^{+2} by complexometry (direct titration method)
11. Estimation of Ca^{+2} by complexometry (substitution titration method)
12. Estimation of Ni^{+2} by complexometry (back titration method)
13. Estimation of Al^{+3} by complexometry (back titration method)

IV. One component Gravimetric Analysis

14. Estimation of Zn^{+2}
15. Estimation of Ba^{+2}

References :

1. Text book of Quantitative Inorganic Analysis, 3rd edition, A.I.Vogel, ELBS (1969)
2. Vogel's text book of Quantitative Inorganic analysis, 4th edition, Jeffery etal, ELBS (1988).
3. Vogel's text book of Quantitative Inorganic Analysis, 6th edition, J.Mendham etal, Pearson education ltd (2002).
4. Practical Inorganic chemistry, G. Marr and B.W.Rockett, Van Nostrand Reinhold (1972).
5. Experimental Inorganic/Physical Chemistry—An Investigative integrated approach to Practical Project work, Mounir A.Malati, Woodhead publishing Ltd., (1999).
6. Advanced experimental Inorganic Chemistry, Ayodhya Singh, Campus books International (2006)
7. Practical Inorganic Chemistry, G. Pass & H. Sutcliffe, University science books (1999)

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Paper CH 152P: Organic Chemistry Lab-I: 4 hrs / week

Synthesis of the following compounds and monitoring the progress of chemical reactions by TLC:

1. p-Bromoacetanilide (using Ceric ammonium nitrate and KBr)
2. p-bromoacetanilide (using bromine)
3. p-Bromoaniline
4. Tetrahydrocarbazole
5. 7-hydroxy-4-methylcoumarin
6. m-dinitrobenzene
7. m-nitroaniline
8. Hippuric acid
9. Anthracene-maleic anhydride adduct
10. Phthalimide.
11. Deamination

References.

1. Text book of practical organic chemistry, Vogel
2. Text book of practical organic chemistry, Mann and Saunders.

Paper 153P: Physical Chemistry Lab-I: 4 hrs / week

Physical properties:

1. Determination of density, surface tension and viscosity of liquids

Distribution:

2. Distribution of acetic acid between n-butanol and water
3. Distribution of iodine between Cyclohexane/n-Hexane and water

Chemical kinetics:

4. Acid-catalyzed hydrolysis of methyl acetate
5. Peroxydisulphate- I- reaction (overall order)
6. Oxidation of iodide ion by hydrogen peroxide- iodine clock reaction

Conductometry:

7. Titration of strong acid vs strong base
8. Titration of weak acid vs strong base
9. Determination of cell constant
10. Determination of dissociation constant of a weak acid

Potentiometry:

11. Titration of strong acid vs strong base
12. Titration of weak acid vs strong base
13. Determination of dissociation constant of a weak acid
14. Determination of single electrode potential

Polarimetry:

15. Determination of specific rotation of sucrose
16. Acid-catalyzed hydrolysis of sucrose (inversion of sucrose)

Adsorption and others:

17. Adsorption of acetic acid on animal charcoal or silica gel
18. Determination of critical solution temperature of phenol-water system
19. Effect of added electrolyte on the CST of phenol-water system

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References:

1. Senior Practical Physical Chemistry: B.D. Khosla, V.C. Garg and A. Khosla
2. Experimental Physical Chemistry: V. Athawale and P. Mathur.
3. Practical Physical Chemistry: B. Vishwanathan and P.S. Raghavan.
4. Practical in Physical Chemistry: P.S. Sindhu
5. Advanced Practical Physical chemistr: J.B.Yadav
6. Vogel Text book of Quantitative Analysis, 6th edition, Pearson education Ltd. 2002.

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MAHATMA GANDHI UNIVERSITY, NALGONDA
DEPARTMENT OF CHEMISTRY
(Effective from the academic year 2023-2024)

SEMESTER –II

Paper-I: CH 201T (INORGANIC CHEMISTRY)

IC 05: Reaction mechanisms of transition metal complexes

IC 06: Bonding in metal complexes-II

IC 07: Metal Clusters

IC 08: Bioinorganic Chemistry

IC-05: Reaction mechanisms of transition metal complexes:

15 Hrs

Ligand substitution reactions: Energy profile of a reaction, transition state or activated complex. Types of substitution reactions: (SE, SN, SN¹, SN²). Langford-Gray classification: A mechanism, D- Mechanism, I-Mechanism I_a, I_d, and Intimate mechanism.

Ligand substitution reactions in octahedral complexes: Aquation or acid hydrolysis reactions, factors affecting acid hydrolysis. base Hydrolysis, conjugate base mechanism, evidences in favour of SN¹CB Mechanism. Substitution reactions without breaking metal-ligand bond. Anation reactions.

Ligand Substitution reactions in square-planar complexes: Mechanism of substitution in square-planar complexes, trans-effect, trans-influence, Grienberg's polarization theory and π -bonding theory, Applications of trans-effect in synthesis of Pt (II) complexes.

Electron transfer reactions (or oxidation-reduction reactions) in coordination compounds: Mechanism of one-electron transfer reactions, atom (or group) transfer or inner sphere mechanism, direct electron transfer or outer sphere mechanism, Factors affecting direct electron transfer reactions, Cross reactions and Marcus-Hush theory.

IC-06: Bonding in Metal Complexes – II:

15 Hrs

Free ion terms and Energy levels: Configurations, terms, states and microstates. Calculation of the number of microstates for pⁿ and dⁿ configurations. Vector coupling of orbital angular momenta, spin angular momentum. Spin orbit coupling: L-S (Russel-Saunders) coupling scheme, j-j coupling scheme. Determination of terms for p¹, p², d¹ and d² configurations of metal ions. Hole formalism. Energy ordering of terms (Hund's rules). Inter – electron repulsion parameters (Racah parameters). Spin-orbital coupling parameters. Effect of weak cubic crystal fields on S, P, D and F terms. Orgel diagrams for (i) d¹, d⁴, d⁶, d⁹ (ii) d², d³, d⁷, d⁸ (iii) d⁵ octahedral and tetrahedral complexes.

IC-07: Metal Clusters:

15 Hrs

Carbonyl clusters: Factors favouring Metal-Metal bonding – Classification of Clusters – Low Nuclearity Clusters : M₃ and M₄ clusters , structural patterns in M₃(CO)₁₂ (M=Fe,Ru,Os) and M₄(CO)₁₂ (M=Co,Rh,Ir) Clusters-. Metal carbonyl scrambling – High Nuclearity clusters M₅,M₆,M₇,M₈ and M₁₀ Clusters-, Polyhedral skeletal electron pair theory and Total

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Electron Count theory – Wades rules – Capping rule – Structural patterns in $[\text{Os}_6(\text{CO})_{18}]^{2-}$, $[\text{Rh}_6(\text{CO})_{16}]$, $[\text{Os}_7(\text{CO})_{21}]$, $[\text{Rh}_7(\text{CO})_{16}]^{3-}$, $[\text{Os}_8(\text{CO})_{22}]^{2-}$, $[\text{Os}_{10}\text{C}(\text{CO})_{24}]^{2-}$ and $[\text{Ni}_5(\text{CO})_{12}]^{2-}$.
 Metal Halide clusters: Major structural types in Dinuclear Metal-Metal systems – Edge sharing Biocahedra, Face sharing Biocahedra, Tetragonal prismatic and Trigonal antiprismatic structures -. Structure and bonding in $[\text{Re}_2\text{Cl}_8]^{2-}$ and Octahedral halides of $[\text{Mo}_6(\text{Cl})_8]^{4+}$ and $[\text{Nb}_6(\text{Cl})_{12}]^{2+}$. Trinuclear halides of Re(III). Hoffman's Isolobal analogy and its Structural implications.

15 Hrs

IC-08: Bioinorganic Chemistry:

Transport of Oxygen: Haemoglobin, Myoglobin, Hemerythrin and Hemocyanin.
 Transport of Electrons: Iron-Sulphur Proteins: Rubredoxins and Ferredoxins (2Fe, 3Fe, 4Fe, 8Fe Proteins)-High Potential Iron-Sulphur Proteins –Structural and Spectral features of Iron-Sulphur Proteins Electron-transport by Cytochromes, Azurin and Plastocyanin -Importance of Structures of Azurin and Plastocyanin facilitating Rapid Electron Transport, acotinase-Fe-S enzyme.

Transport and Storage of Metal Ions: Iron-Transport by Transferrin and Siderophores – Ferritin in Iron Storage -Transport of Na^+ and K^+ across Cell Membranes by $\text{Na}^+ \text{K}^+ \text{ATPase}$ - Transport of Calcium across Sarcoplasmic Reticulum by $\text{Ca}^{2+} \text{-ATPase}$.
 Vitamin B6 model systems: Forms of vitamin B6 with structures. Reaction mechanisms of (1) Transamination (2) Decarboxylation and (3) Dealdolization in presence of metal ions.

References:

1. Inorganic reaction mechanisms, M.L.Tobe & John Burgess, Wesley Longman (1999)
2. Reaction mechanisms in metal complexes, K.Veera Reddy, New age publishers (2020)
3. Mechanisms of Reactions at Transition Metal Sites, Richard A Henderson, Oxford Science Primers, London (1993).
4. Mechanisms of inorganic reactions, F.Basalo & R.G.Pearson, 2nd Edition, John Wiley and Sons, New York (1967)
5. Inorganic reaction mechanisms, R.K.Sharma, Discovery publishing house (2007)
6. Advanced Inorganic Chemistry. F.A.Cotton, G.Wilkinson, C.A.Murillo and M.Bochmann, 6th Edition, Wiley Interscience, N.Y (1999)
7. Principles of Inorganic Chemistry, Puri, Sharma, Kalia, 33rd Edition, Vishal Publications (2022).
8. Concise coordination chemistry, R Gopalan & V Ramalingam, Vikas publishing house Pvt. Ltd., (2008)
9. Selected topics in inorganic chemistry, Wahid U. Malik, G.D. Tuli & R.D. Madan.Chand & Co Ltd (1998)
10. Concise Inorganic Chemistry, J.D.Lee, 5th Edition, Chapman & Hall (2016).
11. Symmetry and Spectroscopy of Molecules. K.Veera Reddy, New Age International (P) Ltd. 2022.
12. Inorganic Chemistry, J.E. Huheey, K.A.Keiter and R.L.Keiter 4 th Edition Harper Cottens College Publications (1993).
13. The Chemistry of Metal Cluster Complexes. D.F.Shriver, H.D.Kaerz and R.D.Adams (Eds), VCH, NY (1990).

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14. Bioinorganic Chemistry, Bertini, Gray, Lippard and Valentine, University Science Books, California USA 1994.
15. Principles of Bioinorganic Chemistry, S.J. Lippard and M. Berg University Science Books California 1994.
16. Biological Chemistry of Elements, J.J.R. Franstodasilva and R.J.P. Williams Oxford University Press 1991.
17. Metal Ions in Biological Systems (Series), Ed. H. Sigel Marcel Dekkar, New York

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Paper-II: CH 202T (ORGANIC CHEMISTRY)

OC-05: Synthetic Strategies

OC-06: Reaction mechanism-II

OC-07: Reactive intermediates and Molecular rearrangements

OC-08: Natural products (Terpenoids and Alkaloids)

OC-05: Synthetic Strategies

15 Hrs

Introduction to terminology: Target, Disconnection Retrosynthesis, Synthons, Synthetic equivalent, Types of Strategies: functional group inter conversion (FGI), functional group elimination (FGE) Criteria for selection of target, Types of Synthesis - Linear and convergent synthesis. Retrosynthetic analysis and synthesis involving chemoselectivity, regioselectivity, reversal of polarity, order of events in synthesis. Retrosynthesis of Salbutamol and Dinocap. Introduction to one group C-C and C-X disconnections, One group C-C disconnections in alcohols, carbonyl compounds, ethers and sulphides.

Introduction to two group C-C and C-X disconnections- two group C-X disconnections in 1,1-difunctionalised, 1,2-difunctionalised and 1,3-difunctionalised 1,5-difunctionalised compounds, Control in carbonyl condensations, explanation by taking examples oxamide. Strategic bond-definition, choosing disconnection/guidelines for disconnections. Other approaches to retrosynthesis-biomimetic approach (johnsons polyene cyclisation), and retro mass spectral fragmentation; application of the strategies to the synthesis of (+) Disparlure.

OC-06: Reaction mechanism-II

15 Hrs

Nucleophilic Aromatic substitution: Aromatic Nucleophilic substitution: $SN_1(Ar)$, $SN_2(Ar)$, and benzyne mechanisms; evidence for the structure of benzyne. Von Richter rearrangement. Definition and types of ambident nucleophiles.

Neighboring group participation: Criteria for determining the participation of neighboring group. Enhanced reaction rates, retention of configuration, isotopic labeling and cyclic intermediates. Neighboring group participation involving Halogens, Oxygen, Sulphur, Nitrogen, Aryl, Cycloalkyl groups, σ and π - bonds. Introduction to nonclassical carbocations.

Electrophilic substitution at saturated carbon and single electron transfer reactions.

Mechanism of aliphatic electrophilic substitution. SE_1 , SE_2 , and SE_i . SET mechanism.

OC-07: Reactive intermediates and Molecular rearrangements

15 Hrs

Reactive Intermediates: Generation, detection, structure, stability and reactions of carbocations, carbanions, carbenes, nitrenes and free radicals.

Molecular rearrangements: Definition and classification. Molecular rearrangements involving 1) electron deficient carbon: Wagner- Meerwein, Pinacol-Pinacolone, Allylic and Wolf rearrangement. 2) electron deficient Nitrogen: Hofmann, Lossen, Curtius, Schmidt and Beckmann rearrangements 3) electron deficient Oxygen: Baeyer-Villiger oxidation. 4) Base catalysed rearrangements: Benzilic acid, Favorski, Transannular, Sommelet-Hauser and Smiles rearrangement.

OC-08: Natural products-I (Terpenoids and Alkaloids)

15 Hrs

Importance of natural products as drugs. Isolation of natural products by steam distillation, solvent extraction and chemical methods. General methods in the structure determination of terpenes. Isoprene rule.

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Structure determination and synthesis of α -terpeniol and camphor. Biogenesis of monoterpenes. Structure determination and synthesis of β -carotene. General methods of structure determination of alkaloids. Structure determination and synthesis of papaverine and quinine.

References:

1. Organic synthesis-the disconnection approach-S Warren
2. Organic synthesis-C Willis and M Willis
3. Problems on organic synthesis-Stuart Warren
4. Advanced Organic Chemistry by Jerry March
5. Mechanism and Structure in Organic Chemistry S. Mukerjee
6. Organic chemistry Vol. I and II by I.L. Finar
7. Comprehensive organic chemistry Vol.5 D.H.R. Barton and W.D..Ollis
8. Organic Chemistry, Vol. 2 by I.L. Finar.
9. Chemistry of Natural Products by Bhat, Nagasampangi and Siva Kumar.
10. Alkaloids by K.W. Bentley.
11. Steroids and Terpenoids by Bentley.

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Paper-III: CH 203T (PHYSICAL CHEMISTRY)

PC-05: Thermodynamics-II

PC-06: Photochemistry

PC-07: Quantum Chemistry-II

PC-08: Solid State Chemistry

PC-05: Thermodynamics-II

15 Hrs

Solutions: Specifying the Solution composition. Partial molar properties-significance. Relation between solution volume and partial molar volume. Measurement of partial molar volumes- slope and intercept methods. The chemical potential. Variation of chemical potential with T and P. Gibbs-Duhem equation-derivation and significance Ideal solutions. Thermodynamic properties of ideal solutions. Mixing quantities. Vapour pressure-Raoult's law. Thermodynamic properties of ideally dilute solutions. Vapour pressure- Henry's law.

Nonideal systems. Concept of fugacity, fugacity coefficient. Determination of fugacity. Nonideal solutions. Activities and activity coefficients. Standard-state conventions for nonideal solutions. Determination of activity coefficients from vapour pressure measurements. Activity coefficients of nonvolatile solutes using Gibbs-Duhem equation. Multicomponent phase equilibrium: Vapour pressure lowering, freezing point depression and boiling point elevation

PC-06: Photochemistry

15 Hrs

Electronic transitions in molecules. The Franck Condon principle. Electronically excited molecules- singlet and triplet states. Radiative life times of excited states-theoretical treatment. Measured lifetimes. Quantum yield and its determination. Actinometry-ferrioxalate and uranyl oxalate actinometers-problems. Derivation of fluorescence and phosphorescence quantum yields. E-type delayed fluorescence-evaluation of triplet energy splitting(ΔE_{ST}). Photophysical processes, photophysical kinetics of unimolecular reactions. Calculation of rate constants of various photophysical processes-problems, State diagrams Photochemical primary processes. Types of photochemical reactions- electron transfer, photodissociation, addition, abstraction, oxidation and isomerization reactions with examples. Effect of light intensity on the rates of photochemical reactions. Photosensitization. Quenching-Stern Volmer equation. Experimental set up of a photochemical reaction. Introduction to fast reactions- Principle of flash photolysis.

PC-07: Quantum Chemistry-II

15 Hrs

Particle in a box- one dimensional and three dimensional. Plots of ψ^2 and ψ -discussion. Degeneracy of energy levels. Comparison of classical and quantum mechanical particles. Calculations using wave functions of the particle in a box-orthogonality, measurability of energy, position and momentum, average values and probabilities. Application to the spectra of conjugated molecules.

Cartesian, Polar and spherical polar coordinates and their interrelations *Schrodinger equation for the hydrogen atom-* separation into three equations. Hydrogen like wave functions. Radial and angular functions. Quantum numbers n, l and m and their importance. The radial distribution functions. Hydrogen like orbitals and their representation. Polar plots, contour plots and boundary diagrams. *Many electron systems.* Approximate methods. The variation method-variation theorem and its proof. Trial variation function and variation integral.

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Examples of variational calculations. Particle in a box. Construction of trial function by the method of linear combinations. Variation parameters. Secular equations and secular determinant.

Bonding in molecules. Molecular orbital theory-basic ideas. Construction of MOs by LCAO, H₂⁺ ion. The variation integral for H₂⁺ ion. Detailed calculation of Wave functions and energies for the bonding and antibonding MOs. Physical picture of bonding and antibonding wave functions. Energy diagram. The MO and VB wave functions for H₂ molecule and their comparison.

PC-08: Solid State Chemistry

15 Hrs

Electronic properties of metals, insulators and semi-conductors: Electronic structure of solids, Band theory, band structure of metals, insulators and semi-conductors. Electrons, holes and Excitons. The temperature dependence of conductivity of extrinsic semi-conductors. Photo conductivity and photovoltaic effect – p-n junctions.

Superconductivity: Occurrence of superconductivity. Destruction of superconductivity by magnetic fields – Meissner effect. Types of superconductors. Theories of super conductivity –BCS theory.

High temperature superconductors: Structure of defect perovskites. High T_c superconductivity in cuprates. Phase diagram of Y-Ba-Cu-O system. Crystal structure of YBa₂Cu₃O_{7-x}. Preparation of 1-2-3 materials. Origin of high T_c superconductivity.

Nanoparticles and their applications:

Introduction to nanoparticles. Reduced dimensionality in solids – zero dimensional systems, fullerenes, quantum dots. One dimensional system, carbon nano tubes, preparation of nano particles –top down and bottom up methods. Preparation of nanomaterials- – sol gel methods, and chemical vapour deposition method; thermolysis. Characterization of nanoparticles – experimental methods – powder X-ray diffraction, transmission electron microscopy (TEM), and atomic force microscopy (AFM) (detailed theory and instrumentation are not required, working principle & block diagram). Optical properties of nanoparticles, Applications of nanoparticles.

References:

1. Atkin's Physical Chemistry, Peter Atkins and Julio de Paula, Oxford University press
2. Physical Chemistry, Ira N. Levine, McGraw Hill
3. Physical Chemistry-A Molecular approach, D.A. McQuarrie and J.D. Simon, Viva Books Pvt Ltd
4. Molecular Thermodynamics, D.A. McQuarrie and J.D. Simon, University Science Books
5. Quantum Chemistry, Ira N. Levine, Prentice Hall
6. Introduction to Quantum Chemistry, A.K. Chandra, Tata McGraw Hill
7. Introduction to Solids, Leonid V. Azaroff, Tata McGraw Hill
8. Solid state Chemistry, D.K. Chakrabarthy, New Age International
9. Solid state Chemistry and its applications, A.R. West, Plenum.
10. Fundamentals of Photochemistry, K.K.Rohtagi-Mukherji, Wiley-Eastern
11. Molecular Photochemistry, N.J. Turro, Benjamin

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12. Photochemistry, R.P.Kundall and A. Gilbert, Thomson Nelson
13. Essentials of Molecular Photochemistry by A. Gilbert and J. Baggott, Blackwell Scientific Publications.
14. Organic Photochemistry by J.M.Coxon and B.Halton, Cambridge University press.
15. Introductory Photochemistry by A.Cox and T.J.Kemp. McGraw-Hill, London.
16. Principles of the Solid State, H. V. Keer, New Age International

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Paper-IV: CH 204 T (ANALYTICAL TECHNIQUES and SPECTROSCOPY-II)

ASP-05: Electro analytical Techniques

ASP-06: NMR- II

ASP-07: Mass Spectrometry

ASP-08: Photoelectron & ESR spectroscopy

ASP-05: Electro Analytical Techniques

15 Hrs

- a) Types and Classification of Electro analytical Methods.
- i) Potentiometry- Types of electrodes, Hydrogen gas, Calomel, Quinhydrone and glass electrodes. Determination of pH. Potentiometric titrations.
- ii) Conductometry – Definition of terms – conductivity, specific conductivity, cell constant. Mobility of ions, Conductometric titrations.
- b) D.C Polarography: Dropping mercury electrode- Instrumentation-polarogram. Types of Currents: Residual, Migration, Limiting. Two and Three electrode assemblies. Ilkovic equation (derivation not necessary) and its consequences. Types of limiting Currents: Adsorption, Diffusion, Kinetic. Applications of polarography in qualitative and quantitative analysis. Analysis of mixtures. Application to inorganic and organic compounds. Determination of stability constants of complexes.
- c) Brief account of following techniques and their advantages over conventional d.c. polarography.
- (i) A.C. polarography (ii) Square-wave polarography (iii) Pulse polarography (iv) Differential pulse polarography
- d) Amperometric titrations: Principle, Instrumentation. Types and applications of amperometric titrations. Determination of SO_4^{2-} , metal ions viz., Mg^{2+} , Zn^{2+} , Cu^{2+} and other substances.
- e) Cyclic Voltammetry: Principle, instrumentation, reversible and irreversible cyclic voltammograms. Applications. Cyclic voltammetric study of insecticide parathion.

ASP 06: : NMR spectroscopy-II (^1H , ^{19}F and ^{31}P NMR)

15 Hrs

^1H , ^{19}F and ^{31}P and solid state NMR spectroscopy: First order and non-first order spectra e.g., AX, AX₂, AX₃, A₂X₃, AMX and AB, ABC, Simplification of complex spectra: increased field strength, deuterium exchange, Lanthanide shift reagents and double resonance techniques. Discrimination of enantiomers by use of chiral NMR solvents (CSAs), chiral lanthanide shift reagents and Mosher's acid. Nuclear Overhauser enhancement (NOE).

Fluxional molecules- bullvalene, $[\eta^1\text{-C}_5\text{H}_5\text{M}]$, $[\eta^5\text{-(C}_5\text{H}_5)_2\text{Ti}\eta^1\text{-(C}_5\text{H}_5)_2]$ and $[\eta^4\text{-C}_8\text{H}_8\text{Ru(CO)}_3]$.

^{19}F -NMR spectroscopy: ^{19}F chemical shifts, coupling constants. Applications of ^{19}F -NMR involving coupling with ^{19}F , ^1H and ^{31}P : 1,2-dichloro-1,1-difluoro ethane, BrF_5 , SF_4 , PF_5 , ClF_3 , IF_5 , $\text{CF}_3\text{CH}_2\text{OH}$.

^{31}P -NMR spectroscopy: ^{31}P chemical shifts, coupling constants. Applications of ^{31}P NMR involving coupling with ^{31}P , ^{19}F , ^1H and ^{13}C : ATP, Ph_3PSe , P_4S_3 , $\text{P(OCH}_3)_3$, H_3PO_4 , H_3PO_3 , H_3PO_2 , HPF_2 , PF_6^- , PH_3 , $[\text{Rh(PPH}_3)_3\text{Cl}]$ (Rh: I=1/2) Introduction to solid state NMR: Magic angle spinning (MAS). Applications of solid state NMR.

ASP 07: Mass spectrometry-I

15 Hrs

Origin of mass spectrum, Principles of EI mass spectrometer. Types of fragments: odd electron and even electron containing neutral and charged species, Nitrogen rule, Isotopic

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peaks, determination of molecular formula, metastable ion peaks. High resolution mass spectrometry. Principles of ion production techniques such as EI, CI, FI and FD methods and mass analysers such as time of flight, ion trap and quadrupole analyzer. Fast Atom Bombardment (FAB), Secondary Ion Mass (SIM) spectrometry and Californium plasma desorption techniques. Principle of Electron Spray Ionization (ESI) mass spectrometry, Matrix Assisted Laser Desorption Ionization (MALDI) mass spectrometry, GC-MS and LC-MS.

ASP-08: Photoelectron & ESR spectroscopy

15 Hrs

Photoelectron Spectroscopy

Principle and Instrumentation, Types of Photoelectron Spectroscopy – UPS & XPS Binding Energies, Koopman's Theorem, Chemical Shifts. Photoelectron Spectra of Simple Molecules: N₂, O₂, F₂, CO, HF, NH₃ and H₂O – Vibrational Structure of PES Bands, Potential energy curves, Interpretation of Vibrational spectral data for ionized (M⁺) species, Prediction of Nature of Molecular Orbitals. ESCA in qualitative analysis, Principles of Auger electron spectroscopy.

Electron Spin Resonance

Introduction, principle, instrumentation, selection rules, interpretation of Lande's factor 'g'. Hyperfine and super hyperfine Coupling. Anisotropy in 'g' values and hyperfine coupling constants. Zero field splitting, Kramer's degeneracy, quadrupolar interactions. Study of free radicals and transition metal complexes. Evidence for covalency in complexes, ex. Cu (II) Bissalicylaldimine, Bis-acetylacetonovanadyl(II) and hexachloroiridium(IV) complexes.

References:

1. Spectroscopic identification of organic compounds by R.M. Silverstein and F.X. Webster.
2. Organic spectroscopy by William Kemp
3. Mass Spectrometry for Chemists and biochemists by M. Rose and R.A. W. Johnstone
4. Spectroscopic methods in organic chemistry by D.H. Williams and I. Fleming
5. Practical Pharmaceutical Chemistry by A. H. Beckett and J.B. Stenlake
6. Biological Mass Spectrometry by A.L. Burlingame
7. Principles and Practice of Biological Mass Spectrometry by Chhabil Das
8. Spectroscopic identification of organic compounds by R.M.Silverstein. G.C.Bassler and T.E.Morrill
9. NMR-A multinuclear introduction by William Kemp
10. Stereochemistry of Carbon compounds by Ernest L Eliel / Samuel H. Wilen
11. Principles of Polarography, Heyrovsky.
12. Principles of Polarography, Kapoor.
13. Modern Electroanalytical methods, edited by C.Charlot, Elsevier Company.
14. Principles of Instrumental analysis, Skoog, Holler and Nieman, Harcourt Asia PTE Ltd.
15. Analytical Chemistry-An Introduction, Skoog, West, Holler and Crouch, Saunders College Publishing.
16. Principles of Instrumental Analysis, Skoog and Leary, Saunders College Publishing.
17. International series of Monographs, Vol. 53: Photoelectron Spectroscopy, Edited by D. Beckerand D. Betteridge 1972.
18. Structural methods in Inorganic Chemistry, E.A.V. Ebsworth.

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Paper CH 251P : Inorganic Chemistry Lab-II: 4 hrs/ week

I. Preparation of complexes:

1. Mercury tetrathiocyanatocobalt(II)
2. Chloropentamminecobalt(III) chloride
3. Tetramminecopper(II) sulphate

II. Titrimetric Analysis of two ions in a mixture

4. Estimation of Pb^{2+} and Ca^{2+}
5. Estimation of Zn^{2+} and Mg^{2+}
6. Estimation of Mg^{2+} and Mn^{2+}

III. Analysis of Two component mixtures

- 7,8. Separation of Ag^+ and Ca^{2+} in a mixture and estimation of Ag^+ (gravimetric) and Ca^{2+} (volumetric)
- 9,10. Separation of Cu^{2+} and Ni^{2+} in a mixture and estimation of Ni^{2+} (gravimetric) and Cu^{2+} (volumetric)
- 11,12. Separation of Fe^{3+} and Al^{3+} in a mixture and estimation of Fe^{3+} (volumetric) and Al^{3+} (gravimetric)

IV. Analysis of three component mixtures:

13. Separation of (Ni^{2+} and Cu^{2+}) from Mg^{2+} in the given mixture and estimation of Mg^{2+} gravimetrically

V. Ion exchange methods of analysis:

14. Determination of capacity of an ion exchange resin.
15. Separation of Mg^{2+} and Zn^{2+} on an anion exchange resin and estimation of Mg^{2+} and Zn^{2+}

References:

1. Text book of Quantitative Inorganic Analysis, 3rd edition, A.I.Vogel, ELBS (1969)
2. Vogel's text book of Quantitative Inorganic analysis, 4th edition, Jeffery etal, ELBS (1988)
3. Vogel's text book of Quantitative Inorganic Analysis, 6th edition, J. Mendham etal, Pearson Education Ltd., (2002).
4. Practical Inorganic Chemistry, G.Marr and B.W.Rockett, Van Norstand Reinhold (1972).
5. Experimental Inorganic/Physical Chemistry – An Investigative integrated approach to Practical Project work, Mounir A. Malati, Woodhead publishing ltd.,(1999).
6. Advanced experimental Inorganic Chemistry, Ayodhya Singh, Campus books International (2006)
7. Practical Inorganic Chemistry, G.Pass & H. Sutchiffe, University Science books(1999).

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Paper CH 252P: Organic Chemistry Lab-II: 4 hrs / week

Identification of organic compounds, systematic qualitative analysis: Physical data BP / MP, Ignition test, Lassaigne test – Nitrogen, Sulphur and halogens, solubility classification. Functional groups tests, Preparation of crystalline derivative and determination of their m.p.s and reference to literature to identify the compounds.

A minimum of 10 compounds covering different functional groups and solubility pattern.

1. Glucose
2. Benzoic acid
3. 2-Chloro benzoic acid
4. Anisic acid
5. p-Nitrobenzoic acid
6. p-Cresol
7. p-Chlorophenol
8. β -Naphthol
9. Aniline
10. o/m/p-Chloroanilines
11. N-methylaniline / N-ethylaniline
12. N, N-dimethylaniline
13. Benzamide
14. Acetanilide
15. Benzaldehyde
16. Anisaldehyde
17. Acetophenone
18. Benzophenone
19. Ethylbenzoate
20. Methylbenzoate
21. Nitrobenzene
22. Chlorobenzene
23. Bromobenzene
24. Naphthalene
25. Biphenyl
26. Anthracene.

Identification of unknown organic compounds from their IR, UV, ^1H NMR and Mass Spectral data:

Analysis of recorded spectra of compounds belonging to i) alkynes, ii) alcohols and phenols iii) aldehydes and ketones iv) carboxylic acids, v) esters vi) acid amides and vii) primary and secondary amines.

References:

1. Text book of practical organic chemistry, Vogel
2. Text book of practical organic chemistry, Mann and Saunders.
3. Spectral identification of organic compounds Bassler, Silverstein 5th Edition.

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P. S. Reddy, M. S. Reddy, S. S. Reddy

Paper CH 253P: Physical Chemistry Lab-II: 4 hrs /week

Distribution:

- 1) Distribution of I_2 between Cyclohexane/n-Hexane and aq.KI solution- calculation of equilibrium constant.
- 2) Study of complex formation between ammonia and metal ion

Chemical Kinetics

- 1) Stoichiometry of peroxydisulphide- iodide reaction
- 2) Peroxydisulphide- iodide reaction: order w.r.t $[I^-]$ by isolation method
- 3) Peroxydisulphide- iodide reaction: order w.r.t $[S_2O_8^{2-}]$ by initial rate method

Conductometry:

- 1) Titration of a mixture of strong and weak acids vs strong base
- 2) Determination of the hydrolysis constant of aniline hydrochloride
- 3) Determination of solubility product

Potentiometry:

- 1) Titration of Fe^{+2} vs $Cr_2O_7^{-2}$ (redox titration)
- 2) Titration of Cl^- vs Ag^+ (precipitation titration)
- 3) Determination of solubility product

Polarimetry:

- 1) Determination of specific rotation of glucose and fructose
- 2) Enzyme catalyzed inversion of sucrose

Colorimetry:

- 1) Verification of Beer's law and calculation of molar absorption coefficient using $CuSO_4$ and $KMnO_4$ solutions

pH metry:

- 1) Calibration of a pH meter and measurement of pH of different solutions
- 2) Preparation of phosphate buffers

Solutions:

- 1) Determination of molecular weight of a nonvolatile substance by cryoscopic method
- 2) Determination of degree of dissociation by cryoscopic method
- 3) Study of surface tension-concentration relationship for solutions (Gibbs equation)

References:

1. Senior Practical Physical Chemistry: B.D. Khosla, V.C. Garg and A. Khosla
2. Experimental Physical Chemistry: V. Athawale and P. Mathur.
3. Practical Physical Chemistry: B. Vishwanathan and P.S. Raghavan.
4. Practical in Physical Chemistry: P.S. Sindhu
5. Advanced Practical Physical chemistr: J.B. Yadav
6. Vogel Text book of Quantitative Analysis, 6th edition, Pearson education Ltd. 2002

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R. Prasad, P. Reddy, K. Reddy, D. Reddy, 24/11/23, Chairperson BOS, M. S. R., S. R., P. Reddy, D. Reddy, 24/11/23, Chairperson BOS