ANDHRA MAHILA SABHA
ARTS & SCIENCE COLLEGE FOR WOMEN
Autonomous - NAAC Re-Accredited,
O.U.Campus, Hyderabad – 500 007

Scheme of Instruction, Evaluation
And Syllabus of
M.Sc (Organic Chemistry)
With effect from Academic Year 2025-2026

Department of Chemistry

DEPARTMENT OF CHEMISTRY

Semester I

Theory/Practicals	Hours/ week	Internal Assessment	Semester Exam	Total	Credits
CHE 401	4	30 marks	70 marks	100 marks	4
CHE 402	4	30 marks	70 marks	100 marks	4
CHE 403	4	30 marks	70 marks	100 marks	4
CHE 404	4	30 marks	70 marks	100 marks	4
CHE 431	4		50 marks	50 marks	2
CHE 432	4		50 marks	50 marks	2
CHE 433	4		50 marks	50 marks	2
CHE 434	4		50 marks	50 marks	2
Total	32			**600 marks**	24

Semester II

Theory/Practicals	Hours/ week	Internal Assessment	Semester Exam	Total	Credits
CHE 451	4	30 marks	70 marks	100 marks	4
CHE 452	4	30 marks	70 marks	100 marks	4
CHE 453	4	30 marks	70 marks	100 marks	4
CHE 454	4	30 marks	70 marks	100 marks	4
CHE 481	4		50 marks	50 marks	2
CHE 482	4		50 marks	50 marks	2
CHE 483	4		50 marks	50 marks	2
CHE 484	4		50 marks	50 marks	2
Total	32			**600 marks**	24

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M.Sc CHEMISTRY SYLLABUS
(Effective from academic year 2025-2026)

SEMESTER –I

Paper 1: CHE 401 (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 h**

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 inmolecular 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), Platonic solids: T_d (CH_4, SiH_4, $[Ni(CO)_4]$), O_h (SF_6, $[PtCl_6]^{2-}$), I_h ($B_{12}H_{12}^{2-}$, C_{60}), 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: **15h**

Crystal Field Theory: Salient features of CFT. d-orbital splitting patterns in regular octahedral, tetrahedral, square planar, tetragonally distorted octahedral, Jahn-Tellar 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 spinel's.

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: **15 h**

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. 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.

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IC-04: Ligational Aspects of Diatomic molecules **15hrs**

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 $[IrCl(PPh_3)_2(CO)(NO)]^+$ and $[RuCl(PPh_3)_2(NO)_2]^+$. Stereo chemical control of valence in $[Co(diars)_2(NO)]^{2+}$ and $[Co(diars)_2(NO)(SCN)]^+$.

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 Os(II) 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, 33rd Edition, Vishal Publications (2022).
10. Metal complexes in Aqueous Solutions, A.E Martell and Robert Hancock, Springer Science (1996)
11. Homogeneous Catalysis by Metal complexes Vol I, M M Taqui Khan and A E Martell, Academic Press NY (1974).

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Paper-II: CHE 402 (Organic Chemistry)
OC-01: Stereochemistry
OC-02: Reaction mechanism-1
OC-03: Conformational analysis (Acyclic systems)
OC-04: Heterocyclic compounds & Natural products

OC-01: Stereochemistry **15 h**

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

Molecular Symmetry & Chirality: Symmetry operations and symmetry elements (Cn & Sn). Criteria for Chirality. Desymmetrization.

Axial, planar and helical chirality: Axially chiral allenes, spiranes, alkylidene cycloalkanes, chiral biaryls, atropisomerism, planar chiral ansa compounds and trans- cyclooctene, helically chiral compounds and their configurational nomenclature.

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

Racemisation and resolution techniques: Racemisation, 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 **15 h**

Electrophilic addition to carbon carbon double bond: Stereo selective 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 E2, E1, E1CB mechanisms. Orientation and stereo selectivity in E2 eliminations. Pyrolytic *syn* elimination and α-elimination.

Determination of reaction mechanism: Determination of reaction mechanism: Product isolation, Structure of intermediates, use of isotopes and crossover experiments. Use of IR and NMR in the investigation of reaction mechanism.

OC-03: Conformational analysis (acyclic systems) **15 h**

Conformational isomerism: Introduction to the concept of dynamic stereochemistry. Conformational diastereoisomers and conformational enantiomers. Study of conformations in ethane and 1,2-disubstituted ethane derivatives like butane, dihalobutanes, halohydrin, ethylene glycol, butane-2, 3-diol amino alcohols and 1,1,2,2-tetrahalobutanes. Klyne-Prelog terminology for conformers and torsion angles

Conformations of unsaturated acyclic compounds: Propylene, Acetaldehyde and Butanone.

Factors affecting the conformational stability and conformational equilibrium: Attractive and repulsive interactions. Use of Physical and Spectral methods in conformational analysis use of dipole moment IR and NMR spectral methods in conformational analysis.

Conformational effects on the stability and reactivity of acyclic diastereoisomers: Steric and stereoelectronic factors-examples. Conformation and reactivity. The Curtin– Hammett principle.

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OC-4: Heterocyclic compounds &Natural products **15 h**

Heterocyclic compounds: Introduction, Nomenclature Synthesis and reactivity of indole, quinoline, isoquinoline, carbazole and acridine.

Natural products: Terpenoids: Isoprene rule. Structure determination and synthesis of α-terpeniol and camphor.

Alkaloids: Structure determination and synthesis of papaverine.

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. The Alkaloids by K.W. Bentley

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Paper III: CHE 403 (PHYSICAL CHEMISTRY)
PC-01: Thermodynamics-I
PC-02: Electrochemistry-I
PC-03: Quantum Chemistry-I
PC-04: Chemical Kinetics-I

PC-01: Thermodynamics-I

15 h

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 changes 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). 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- I

15 h

Electrochemical Cells: Derivation of Nernst equation – problems. Chemical and concentration cells (with and without transference). Liquid junction potential (LJP) – derivation of the expression for LJP – its determination and elimination.
Types of reversible electrodes: (i). Gas electrode, ex: Hydrogen electrode; (ii). Metal-Metal ion electrode, ex: Cu in $CuSO_4$, Zn in $ZnSO_4$; (iii). Metal-insoluble metal salt electrode, ex: calomel electrode, Ag-AgCl electrode; (iv). Redox electrodes, ex: Pt in Fe^{2+}/Fe^{3+}, Quinhydrone electrode; (v). Ion-selective electrodes, ex: H^+ selective-glass electrode, other ion selective electrodes (fluoride, sodium, calcium etc.). Applications of EMF measurements: Solubility product, potentiometric titrations, equilibrium constant measurements, determination of pH using glass electrode. Applications of ion-selective electrodes in medicine (ex: blood electrolyte analysis).
Decomposition potential and its significance. Electrode polarization – its causes and elimination. Concentration over-potential.
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.

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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 h

A brief review of Black body radiation and Planck's quantization- (derivation not required), Wave particle duality and uncertain principle-significance of these for microscopic entities. Emergence of quantum mechanics. Wave mechanics and Schrödinger wave equation.

Operators- Operator algebra. Commutation of operators, linear operators. Complex functions and Hermitian operators. Operators ∇ and ∇^2. Eigenfunctions and eigenvalues. Degeneracy. Linear combination of eigenfunctions. Well behaved, normalized and orthogonal functions.

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.

Particle in a box- one dimensional and three dimensional. Plots of ψ and ψ^2-discussion. Degeneracy of energy levels. Calculations using wave functions of the particle in a box- orthogonality, measurability of energy, position and momentum, average values and probabilities.

Application of particle in 1D-box model to the spectra of conjugated molecules. HOMO-LUMO gaps and relevance to electronic spectroscopy.

PC-04: Chemical Kinetics- I 15 h

Theories of reaction rates: Collision theory and steric factor. Transition state theory. Reaction coordinate, Activated complex, and the transition state. Thermodynamic formulation of transition state theory - Derivation of Eyring equation and interpretation of activation parameters ($\Delta H^{\ddagger}$, $\Delta S^{\ddagger}$, $\Delta G^{\ddagger}$) and their significance.

Unimolecular and Complex reactions: Unimolecular reactions - Lindemann's theory of unimolecular reactions; Complex reactions (all first order type) - Opposing reactions, parallel reactions and consecutive reactions. Chain reactions-general characteristics, steady state treatment. Example- H_2-Br_2 reaction. Derivation of rate law.

Effect of structure on reactivity: Linear free energy relationships, Hammett equation: substituent constant (σ) and reaction constant (ρ); applications and limitations; Taft equation: substituent

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constant (σ^*) and reaction constant (ρ^*); Taft four parameter equation; Numerical problems on Hammett and Taft equations.

Deviations from Hammett correlations: Change of mechanism, resonance effects.

Correlations for nucleophilic substitution correlations: Swain – Scott equation, Edwards equation. Examples from nucleophilic substitution reactions.

Kinetics in solutions: Primary and secondary salt effects. Marcus theory of electron transfer reactions (qualitative discussion with free energy diagrams)-Hammond's postulate (qualitative)

References

1. Atkin's Physical Chemistry, 11e., Peter Atkins and Julio de Paula, Oxford University press, 2018
2. Physical Chemistry, 6e, Ira N. Levine, McGraw Hill Education, 2011
3. Physical Chemistry-A Molecular approach, D.A. McQuarrie and J.D. Simon, Viva Books Pvt. Ltd., 2020.
4. Molecular Thermodynamics, D.A. McQuarrie and J.D. Simon, University Science Books, 1999.
5. An introduction to Electrochemistry, S. Glasstone; East-West Press (Pvt.) Ltd. 2006.
6. Modern Electrochemistry, J. O. M. Bockris & A. K. N. Reddy, Plenum, 2012 reprint.
7. Principles of physical chemistry, 4e, Samuel H. Maron and Carl F. Prutton, Oxford & IBH, 2017
8. Physical Organic Chemistry, 2e, N. S. Isaacs, ELBS, 1995.
9. Elementary Quantum Chemistry, 2e, F. L. Pilar, McGraw Hill, 1990.
10. Quantum Chemistry – D.A. McQuarrie, Viva Publication, 2020
11. Quantum Chemistry, 7e, Ira N. Levine, Prentice Hall, 2013
12. Introduction to Quantum Chemistry, 4e, A.K. Chandra, Tata McGraw Hill, 2017
13. Quantum Chemistry, 6e, R K Prasad, New Age International Pvt Ltd Publishers,2024.
14. Chemical Kinetics and Reaction Mechanisms, 2e, J. H. Espenson, McGraw Hill,1995.
15. Chemical Kinetics, 3e, K.J. Laidler, McGraw Hill, 2003.
16. The Physical Basis of Org. Chemistry by Howard Maskill, Oxford Univ. Press (New York), 1985.
17. Kinetics and Mechanism of Chemical Transformations, J. Rajaraman & J. Kuriacose, McMillan

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Paper-IV: CHE 404 (ANALYTICAL TECHNIQUES and SPECTROSCOPY- I)

ASP 01: Techniques of Chromatography
ASP 02: NMR spectroscopy-I (^{1}H NMR)
ASP 03: Rotational and Vibrational spectroscopy
ASP 04: Electronic spectroscopy

ASP-01: Techniques of Chromatography 15 h

Introduction and general principles: Classification of chromatographic techniques, differential migration rates, partition coefficient(K), retention time, relation between partition coefficient and retention time, capacity factor, selectivity factor. Efficiency of separation: resolution, diffusion, plate theory and rate theory (problems).

Gas Chromatography (GC): Principle and instrumentation, Detectors- TCD, FID, ECD. Derivatization techniques, Pyrolysis Gas Chromatography (PTGC).

High Performance Liquid Chromatography (HPLC): Principle and modes (normal phase, reverse phase), Instrumentation, Detectors - UV detectors, Photodiode array detector, fluorescence detector.

Other Chromatographic methods: Ion exchange chromatography and Size-exclusion chromatography (outline).

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. Pesticide residue analysis of azoxystrobin.

ASP 02: NMR Spectroscopy-I (^{1}H NMR) 15 h

^{1}H 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, germinal and long range, Coupling constants and factors affecting coupling constants.

Applications of ^{1}H NMR spectroscopy: Reaction mechanisms (cyclic bromonium ion, electrophilic and nucleophilic substitutions, carbocations and carbanions), cis-trans isomers, 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). ^{1}H NMR of organic molecules and metal complexes: ethyl acetate, 2- butanone, mesitylene, paracetamol, asprin, ethylbenzoate, benzylacetate, 2-chloro propionic acid, $[HNi(OPEt_3)_4]^+$, $[HRh(CN)_5]$ (Rh I=1/2), $[Pt(acac)_2]$.

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ASP 03: Vibrational Spectroscopy **15 h**

Interaction of electromagnetic radiation with matter. Factors affecting width and intensity of spectral lines.

IR Spectroscopy: Vibrational energy levels of diatomic molecules, selection rules (derivation not required). Calculation of force constant from vibrational frequency. Anharmonic oscillator. Morse potential energy diagram. Fundamental bands, overtones and hot bands, Fermi Resonance.

Vibration rotation spectra of diatomic and poly atomic molecules: Vibration – rotation spectroscopy, P, Q, R branches. Vibration – rotation spectra of polyatomic molecules – linear, symmetric top and asymmetric top molecules. Principles of FTIR.

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 - Numerical problems.

Raman spectroscopy: Classical and quantum theories of Raman effect, Stokes and anti- Stokes lines. Complementary nature of IR and Raman spectra. Pure rotational, vibrational and vibrational – rotational Raman spectra. Selection rules. Depolarization factors of Raman lines and their relevance. Instrumentation and applications of Raman spectroscopy.

ASP 04: Electronic spectroscopy **15 h**

Fundamentals of Electronic spectra: Elementary energy levels of molecules-selection rules for electronic spectra; types of electronic transitions in molecules.

Chromophores and conjugated systems: Conjugated dienes, trienes and polyenes, unsaturated carbonyl compounds, Benzene, mono substituted derivative (Ph-R), di substituted derivative (R-C_6H_4-R) and substituted benzene derivatives (R-C_6H_4-COR), Woodward-Fieser rules.

Extended aromatic and Heterocyclic systems: Polynuclear aromatic compounds (Biphenyl, stilbene, naphthalene, anthracene, phenanthrene and pyrene). Heterocyclic systems.

Charge transfer and solvent or structural effects: Absorption spectra of charge transfer complexes. Solvent and structural influences on absorption maxima, stereochemical factors. Cis-trans isomers, and cross conjugation.

Applications of Electronic Spectroscopy Beer-Lambert law: Principle and applications. Beer's law application to mixture analysis and dissociation constant of a weak acid.

References

1. Fundamentals of Molecular Spectroscopy, 4e, Colin N.Banwell and Elaine M. McCash McGraw Hill 1994.
2. Introduction to Molecular Spectroscopy, G.M. Barrow, McGrawHill
3. Absorption Spectroscopy of Organic Compounds, J.R. Dyer Prentice-Hall of India Pvt.Ltd 1978.
4. Introduction to Spectroscopy, 5e, Pavia Lampman Kriz. Cengage learning, 2014.
5. Pharmaceutical analysis, 2e, Watson Elsevier, 2005.

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6. NMR in Chemistry- A multinuclear introduction, William Kemp, Springer, 1986.
7. Organic Spectroscopy, 2e, William Kemp, Palgrave Macmillan 2019.
8. Spectroscopy of organic compounds, 9e, P.S. Kalsi, New Age International Publishers 2022.
9. Structural methods n Inorganic chemistry, E.A.V Ebsworth, John Wiley & Sons, 1991.
10. Organic Spectroscopy, LDS Yadav, Springer, 2005.
11. Elementary Organic Spectroscopy, 5e,Y.R. Sharma S. Chand Limited, 2013.
12. Molecular Structure and Spectroscopy, 2e, by G Arhuldas, PHI Learning Private Ltd. New Delhi, 2007.
13. Vibrational Spectroscopy: Theory and Applications, 4e, D. N. Sathyanarayana, New Age International, 2024.
14. Modern Spectroscopy, 4e, J. M. Hollas, John Wiley & Sons, 2003.
15. Spectroscopy of inorganic compounds by Jagadamba Singh, Mrityunjay D Pandey and Jaya Singh, Second edition 2024, New Age International (P) Ltd., Publishers.

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Paper CHE 431: Inorganic chemistry Lab course **4 h/week**

I. Preparation of complexes

1. Hexaammine nickel (II) chloride.
2. Tris (acetylacetanato) 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 toPractical 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 CHE 432: Organic Chemistry Lab course **4 h/ week**

Synthesis of the following compounds:

1. p-Bromoacetanilide
2. p-Bromoaniline,
3. 2,4,6- tribromoaniline
4. 1,3,5-Tribromobenzene
5. Tetrahydrocarbazole
6. 7-Hydroxy-4-methyl coumarin
7. m-Dinitrobenzene
8. m-Nitroaniline
9. Hippuric acid
10. Azlactone
11. Anthracene-maleic anhydride adduct
12. 2,4-Dihydroxyacetophenone
13. Phthalimide
14. Anthranilic acid

References

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

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Paper CHE 433 Physical Chemistry Lab course **4 h / week**

I. Data analysis I: Significant figures, Precision and accuracy

II. Chemical kinetics:

1. Acid-catalyzed hydrolysis of methyl acetate both with 1N HCl
2. Acid-catalyzed hydrolysis of methyl acetate both with 2N HCl
3. Peroxydisulphate-I^- reaction (overall order)
4. Oxidation of iodide ion by hydrogen peroxide-Iodine clock reaction.

III. Conductometry:

5. Determination of cell constant
6. Titration of strong acid vs strong base
7. Titration of weak acid vs strong base
8. Determination of dissociation constant of a weak acid

IV. Potentiometry:

9. Titration of strong acid vs strong base
10. Titration of weak acid vs strong base and determination of dissociation constant of a weak acid.
11. Determination of single electrode potential

V. Polarimetry:

12. Determination of specific rotation of sucrose
13. Determination of specific rotation of glucose
14. Determination of specific rotation of fructose

VI. Adsorption:

15. Adsorption of acetic acid on animal charcoal or silica gel

References

1. Senior Practical Physical Chemistry B.D. Khosla, V.C. Garg and A. Khosla; R Chand & Co., 2018.
2. Experimental Physical Chemistry: V. Athawale and P. Mathur, New Age, International 2001..
3. Practical Physical Chemistry: B. Vishwanathan and P.S. Raghavan, Viva Books, 2012.
4. Practical in Physical Chemistry: P.S. Sindhu, Laxmi Publications, 2009.
5. Advanced Practical Physical chemistry: J.B.Yadav, Krishna Prakashan Media, 2016.

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Paper CHE 434: Analytical Chemistry -I Lab course **4 h/week**

I. Applied analysis:

1. Estimation of acetic acid in commercial vinegar by acid base titration method
2. Estimation of iron in cement by dichrometry
3. Estimation of available chlorine in bleaching powder by iodometry
4. Estimation of calcium in calcium tablets by complexometry
5. Estimation of magnesium in talcum powder by complexometry

II. Thin layer chromatography

6. Determination of purity of the compounds prepared in CH 152
7. Monitoring the progress of chemical reactions for any of the two preparations in CH 152

III. Assay of drugs:

8. Aspirin by acid base back-titration method
9. Ibuprofen by acid base titration method
10. Calcium in calcium gluconate by complexometry.

IV. Determination of Physical Properties of Solutions:

11. Determination of molecular weight of a polymer by viscometry
12. Determination of critical solution temperature of phenol-water system
13. Effect of added electrolyte on the CST of phenol-water system

V. Colorimetry

14. Verification of Beer's law and calculation of molar extinction coefficient using $CuSO_4$ solution.
15. Verification of Beer's law and calculation of molar extinction coefficient using $KMnO_4$ solution

References

1. Advanced practical chemistry, R.Mukhopadhyay & P. Chatterjee, NCBA books (2016)
2. Advanced practical inorganic chemistry, Gurdeep Raj, GOEL publishing house (2015)
3. Advanced experimental Inorganic chemistry, Ayodhya Singh, Campus books Int. (2006)
4. Senior Practical Physical Chemistry: B.D. Khosla, V.C. Garg and A. Khosla (2018)
5. Advanced Practical Physical Chemistry: J.B.Yadav, 2016.

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M.Sc CHEMISTRY SYLLABUS
SEMESTER –II

Paper-I: CHE 451 (Inorganic chemistry)

IC 05: Reaction mechanisms of transition metal complexes
IC 06: Bonding in metal complexes-II
IC 07: Metal clusters
IC 08: Bio-coordination chemistry

IC-05: Reaction mechanisms of transition metal complexes: **15 h**

Ligand substitution reactions: Energy profile of a reaction, transition state or activated complex. Types of substitution reactions: (SE, SN, SN^1, SN^2). 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 favor of SN^1CB 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 h**

Free ion terms and Energy levels: Configurations, terms, states and microstates. Calculation of the number of microstates for p^n and d^n 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 p^1,p^2,d^1 and d^2 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) d^1, d^4,d^6, d^9 (ii) d^2,d^3,d^7,d^8 (iii) d^5 octahedral and tetrahedral complexes.

IC-07: Metal Clusters: **15 h**

Metal Clusters: Definition, Factors favoring metal-metal bonding.

Metal carbonyl clusters: Classification of carbonyl clusters. Low nuclearity carbonyl clusters: M_3 and M_4 clusters, structural patterns in $M_3(CO)_{12}$ (M=Fe, Ru, Os) and $M_4(CO)_{12}$ (M=Co, Rh, Ir) clusters. High nuclearity carbonyl clusters: M_5, M_6, M_7, M_8 and M_{10} clusters. Polyhedral skeletal electron pair theory and Total electron count theory. Capping rule. Structural patterns in

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$[Ni_5(CO)_{12}]^{2-}$, $[Os_6(CO)_{18}]^{2-}$, $[Os_7(CO)_{21}]$, $[Os_8(CO)_{22}]^{2-}$ and $[Os_{10}C(CO)_{24}]^{2-}$. Metal carbonyl scrambling, stereo chemical non-rigidity in $[Rh_4(CO)_{12}]$ and $[Fe_2(Cp)_2(CO)_4]$.

Boranes and carboranes: Wade's rules, STYX rule.

Metal Halide clusters: Major structural types in dinuclear Metal-Metal systems – Edge sharing bioctahedra, Face sharing bioctahedra, Tetragonal prismatic and Trigonal antiprismatic structures -. Structure and bonding in $[Re_2Cl_8]^{2-}$ and Octahedral halides of $[Mo_6(Cl)_8]^{4+}$ and $[Nb_6(Cl)_{12}]^{2+}$. Trinuclear halides of Re(III). Hoffman's Isolobal analogy and its Structural implications.

IC-08: Bio-coordination chemistry **15 h**

Metal ions in Biological systems: Brief survey of metal ions in biological systems. Effect of metal ion concentration and its physiological effects. Basic principles in the biological selection of elements.

Oxygen transport and storage: Hemoglobin (Hb) and Myoglobin (Mb): Geometric. electronic and magnetic aspects of Dioxygen binding. Oxygen adsorption isotherms and cooperativity in Hemoglobin and its physiological significance. Role of globin chain. **Hemocynin (Hc) and Hemerythrin (Hr):** Introduction-structure of active sites with oxygen and without oxygen. Comparison of Hemerythrin and Hemocyanin with Hemoglobin.

Photosynthesis: Structural aspects of Chlorophyll. Photo system I and Photo system II.

Vitamin B_6 model systems: Forms of vitamin B_6 with structures. Reaction mechanisms of (1) Transamination (2) Decarboxylation and (3) Dealdolation 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, S.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.

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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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Paper-II: CHE 452 (Organic Chemistry)

OC-05: Reaction mechanism-II

OC-06: Pericyclic reactions-I

OC-07: Photochemistry

OC-08: Reactive intermediates and molecular rearrangements

OC-05: 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.

Neighbouring group participation: Criteria for determining the participation of neighbouring group. Enhanced reaction rates, retention of configuration, isotopic labelling and cyclic intermediates. Neighbouring group participation involving Halogens, Oxygen, Sulphur, Nitrogen, Aryl, Cycloalky l groups, σ and π- bonds. Introduction to nonclassical carbocations.

Electrophilic substitution saturated carbon and single electron transfer reactions.

Mechanism of aliphatic electrophilic sustitution. SE^1, SE^2, and SEi.

OC-06 Pericyclic reactions **15 h.**

Introduction, Classification of pericyclic reactions,

Electrocyclic reactions: con rotation and dis rotation. Electrocyclic closure and opening in 4n and 4n+2 systems.

Cycloaddition reactions: suprafacial and antara facial additions in 4n and4n+2 cycloadditions.

Sigmatropic reactions: [i, j] shifts- suprafacial and antarafacial shifts, Cope and Claisen rearrangement reactions.

Approaches for the interpretation of mechanism of pericyclic reactions: Aromatic Transition States (ATS)/Perturbation Molecular Orbitals (PMO) approach-Concept of Huckel –Mobius aromatic and antiaromatic transition states. Framing Woodward-Hofmann selection rules for all the pericyclic reactions by ATS approach. Solving problems based on ATS approach.

Molecular orbitals: ethylene, 1, 3-butadiene, 1, 3, 5-hexatriene, allyl cation, allyl radical, pentadienyl cation, pentadienyl radical.

Frontier Molecular Orbital (HOMO-LUMO) approach-concept: Framing Woodward-Hofmann selection rules for all the pericyclic reactions by Frontier Molecular Orbital (FMO) approach. Solving problems based on FMO approach.

Conservation of orbital symmetry: (Correlation Diagrams) approach- for electrocylic and cycloadditions & cycloreversions.

OC-07 Photochemistry **15hrs**

Photochemistry: Photochemistry of π-π* transitions: Excited states of alkenes, cis-trans isomerisation, and photo stationary state. Photochemistry of 1,3-butadiene Electrocyclisation and sigmatropic rearrangements, di-π methane rearrangement. Intermolecular reactions, photocycloadditions, photodimeriastion of simple and conjugated olefins. Addition of olefins to α, β-unsaturated carbonyl compounds. Excited states of aromatic compounds, Photoisimerisation of benzene.

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Photochemistry of (n-π*) transitions: Excited states of carbonyl compounds, homolytic cleavage of α- bond, Norrish type I reactions in acyclic and cyclic ketones and strained cycloalkane diones.

Intermolecular abstraction of hydrogen: photoreduction-influence of temperature, solvent, nature of hydrogen donor and structure of the substrate.

Intramolecular abstraction of hydrogen: Norrish type II reactions in ketones, esters and 1,2 diketones, Addition to carbon-carbon multiple bonds, Paterno-Buchi reaction,

Photochemistry of nitrites-Barton reaction.

OC-08: Reactive intermediates and Molecular rearrangements **15 hrs**

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

Molecular rearrangements: Definition and classification. Molecular rearrangements involving 1) electron deficient carbon: Allylic and Wolf rearrangement. 2) electron deficient Nitrogen: Lossen, Curtius and Schmidt rearrangements 3) electron deficient Oxygen: Baeyer-Villiger oxidation. 4) Base catalysed rearrangements: Benzilic acid, Favourski, Transannular, Sommlett-Hauser and Smiles rearrangement.

References :

1. Stereochemistry of Carbon compounds by Ernest L Eliel / Samuel H. Wilen
2. Stereochemistry of organic compounds – Principles and Applications by D Nasipuri
3. The third dimension in organic chemistry, by Alan Bassindale
4. Stereochemistry: Conformation and Mechanism by P S Kalsi
5. Stereochemistry by V M Potapov
6. Advanced Organic Chemistry by Jerry March
7. Mechanism and Structure in Organic Chemistry S. Mukerjee
8. Organic chemistry Vol.I and II by I.L.Finar
9. Comprehensive organic chemistry Vol.5 D.H.R.Barton and W.D..Ollis
10. Molecular Reactions and Photo chemistry by Depuy and Chapman, Prentice Hall, 1972.
11. Essentials of Molecular Photochemistry by A. Gilbert and J. Baggott, Wiley-Blackwell Scientific Publications, 1990.

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Paper III: CHE 453 PHYSICAL CHEMISTRY

PC-05: Thermodynamics-II
PC-06: Photochemistry-I
PC-07: Quantum Chemistry-II
PC-08: Solid State Chemistry

PC-05: Thermodynamics-II

15 h

Solutions: Specifying the composition. Partial molar properties and their 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, Thermodynamics of mixing (ΔG_{mix}, ΔH_{mix}, ΔS_{mix}, ΔV_{mix}), Vapour pressure - Raoult's law. Thermodynamic properties of ideally dilute solutions. Vapour pressure - Henry's law.

Non-ideal systems:

Concept of fugacity and fugacity coefficient (qualitative). Determination of fugacity.

Non ideal solutions. Activities and activity coefficients. Standard-state conventions for non-ideal solutions. Excess functions- definition, significance, typical forms - G^E, H^E, S^E,V^E; Determination of activity coefficients from vapor pressure measurements. Activity coefficients of nonvolatile solutes using Gibbs-Duhem equation.

Multicomponent phase equilibria (colligative properties): Vapor pressure lowering, freezing point depression and boiling point elevation. Derivation of colligative properties with molar mass of solute and their applications. Numerical problems.

PC-06: Photochemistry –I

15 h

Molecular Electronic Transitions: Electronic transitions in molecules, Franck-Condon principle. Singlet and triplet states, formation of excimers and exciplexes. Energy diagrams.

Radiative and non-radiative lifetimes life times of excited states-theoretical treatment. Measured life times.

Quantum yield and Measurement: Definition and determination of quantum yields. Actinometry-ferrioxalate and uranyl oxalate actinometers (with problems). Derivation of fluorescence and phosphorescence quantum yields. E-type and P-type delayed fluorescence-evaluation of triplet energy splitting (ΔE_{ST}).

Photophysical processes and kinetics : Photophysical kinetics of unimolecular reactions. R ate constants of various photophysical processes-problems, Energy level/State diagrams.

Photochemistry: General aspects: *P*rimary photochemical processes. Effect of light intensity on reaction rates. Photosensitization and Quenching-Stern-Volmer equation.

Fast Reactions: Introduction to fast reactions. Principle and applications of flash photolysis.

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PC-07: Quantum Chemistry-II

15 h

Hydrogen atom and Atomic orbitals: Coordinate systems: Cartesian, Polar and spherical polar coordinates, and 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* -meaning and importance. Radial distribution functions. Representation of Hydrogenic orbitals : Polar plots, contour pots and boundary diagrams.

Approximate methods for many electron systems: The variation method-variation theorem and its proof. Trial variation functions and variation integrals, examples of variational calculations for simple systems Particle in a box revisited: 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. LCAO construction of MOs - H_2^+ ion. Variation integral for H_2^+ ion. Detailed calculation of Wave functions and energies for the bonding and antibonding MOs.- physical interpretation. The MO wave function and energies and energy diagram of H_2 molecule. Comparison of MO by LCAO method and Valence bond method models. (detailed calculations not required)

PC-08: Solid State Chemistry

15 h

Electronic properties of solids: Electronic structure of solids, Band theory of metals, insulators and conductors, Fermi level, K space and Brillouin Zones (qualitative no derivation). Electrons, holes and Excitons. Temperature dependence of conductivity in 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 $YBa_2Cu_3O_{7-x}$. Preparation of 1-2-3 materials. Origin of high T_c superconductivity.

Nanoparticles and their applications: Introduction to nanoparticles. Reduced dimensionality in solids: systems with various dimensions -examples.

Preparation of nano particles – top down and bottom-up methods. Preparation of nanomaterials- – sol gel methods (ex: nanotitania, silicagel), chemical vapour deposition method (ex: carbon nanotubes, metal nanoparitcles) and thermolysis (ex: metal nanoparticles from metal complexes/salts). Characterization of nanoparticles – experimental methods: XRD, SEM, TEM, AFM (no instrumentation details, principles only), Optical properties of nanoparticles, Applications of nanoparticles in water purification, catalysis, sensors, cosmetics, drug delivery and diagnosis, energy materials.

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References

1. Physical Chemistry-A Molecular approach, D.A. McQuarrie and J.D. Simon, Viva Books Pvt Ltd. 2011.
2. Elements of Physical Chemistry by Peter Atkins and Julio de Paula, Oxford University Press, 2012
6. Fundamentals of Photochemistry, 4e, K.K.Rohtagi-Mukherji, Wiley-Eastern 2021.
7. Molecular Reactions and Photo chemistry by Depuy and Chapman, Prentice Hall, 1972.
8. Molecular Photochemistry, N.J. Turro, Benjamin publication, 2010.
9. Photochemistry, R.P.Kundall and A. Gilbert, Thomson Nelson
10. Essentials of Molecular Photochemistry by A. Gilbert and J. Baggott, Wiley-Blackwell Scientific Publications, 1990.
11. Organic Photochemistry, 2e, by J.M.Coxon and B.Halton, Cambridge University Press, 2011.
12. Introductory Photochemistry by A.Cox and T.J.Kemp. McGraw-Hill, London, 1971.
13. Quantum Chemistry, D.A. McQuarrie, Viva publication, 2020.
14. Quantum Chemistry, 7e, Ira N. Levine, Prentice Hall, 2013
15. Introduction to Quantum Chemistry, 4e, A.K. Chandra, Tata McGraw Hill, 2017
16. Quantum Chemistry, 6e, R K Prasad, New Age International Pvt Ltd Publishers,2024.
17. Elementary Quantum Chemistry, 2e, F. L. Pilar, McGraw Hill, 1990.
18. Introduction to Solids, Leonid V. Azaroff, McGraw Hill, 1960.
19. Solid state Chemistry, D.K. Chakrabarty, New Age International,2021.
20. Principles of the Solid State, H. V. Keer, New Age International Pvt. Ltd. 2017.
21. The physics and chemistry of solids by Stephen Elliott, John Wiley Publishers, 1998.
22. Nanostructured Materials and Nanotechnology, edited by Hari Singh Nalwa, Acad. Press 2001.
23. Self-Assembled Nanostructures, Jin Zhang, Zhong-lin Wang, Jun Liu, Shaowei Chen & Gan-Yu-Liu, Kluwer Academic/Plenum publishers in 2002, later by Springer US in 2013.
24. Introduction to Nanotechnology, Charles P. Poole Jr, F. J. Owens, Wiley India Pvt. Ltd.,2003.

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Paper-IV: CHE 454 (ANALYTICAL TECHNIQUES and SPECTROSCOPY - II)

ASP-05: Electro and Thermal Analytical Techniques.
ASP-06: NMR- II
ASP-07: Mass Spectroscopy
ASP-08: Photoelectron & ESR spectroscopy

ASP-05: Electro and Thermal Analytical Techniques 15 h

Electroanalytical techniques: Classification of Electro analytical Methods – Potentiometry, conductometry, coulometry, voltammetry, polarography. Scope and applications in modern analysis

Polarography: Principle, Types of polarography: A.C Polarography and D.C Polarography. D.C Polarography – Instrumentation, Dropping mercury electrode (DME), two and three electrode assemblies, polarogram. Types of currents: residual, migration, limiting. Ilkovic equation (statement only) and its consequences. Applications of polarography in - qualitative and quantitative analysis, mixture analysis, inorganic and organic compound analysis. Determination of stability constants of complexes.

Amperometric titrations: Principle and Instrumentation. Types of amperometric titrations. Applications: Determination of SO_4^{2-}, metal ions viz., Mg^{2+}, Zn^{2+}, Cu^{2+} and other analytes.

Cyclic Voltammetry: Principle and instrumentation, Applications. Cyclic voltammetric study of insecticide parathion. HOMO-LUMO calculations of ferrocene

Thermal Analytical techniques: Introduction, overview and types of thermal methods.

Thermogravimetry: Principle, typical thermograms, and applications – decomposition of calcium oxalate, calcium sulphate and silver nitrate,

Differential thermal analysis (DTA): Principle, differential thermogram of sulphur and applications in phase transitions and purity studies,

Differential scanning calorimetry (DSC): Principle and distinction from DTA. Applications- determination of glass transition temperatures and heat capacities of PVC and Bakelite.

ASP 06: NMR Spectroscopy-II (^1H, ^{13}C, ^{19}F and ^{31}P NMR) 15 h

^1H, ^{19}F, ^{31}P and solid state NMR spectroscopy: First order and non-first order spectra e.g., AX, AX_2, AX_3, A_2X_3, 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).

^{13}C NMR: ^{13}C chemical shifts, coupling constants. Fluxional molecules bullvalene, [η^1-C_5H_5M], $Cp_2Fe_2(CO)_4$, [η^5-$(C_5H_5)_2Ti\eta^1$-$(C_5H_5)_2$], and [η^4-$C_8H_8Ru(CO)_3$].

^{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, CF_3CH_2OH

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^{31}P NMR spectroscopy: ^{31}P chemical shifts, coupling constants. Applications of ^{31}P NMR involving coupling with ^{31}P, ^{19}F, ^{1}H and ^{13}C: ATP, Ph_3PSe, P_4S_3, H_3PO_4, H_3PO_3, H_3PO_2, HPF_2, PF_6^-, PH_3, [Rh $(PPh_3)_3Cl$] (Rh I=1/2)

Introduction to solid state NMR: Magic angle spinning (MAS). Applications of solid state NMR.

ASP 07: Mass Spectrometry **15 h**

Origin of mass spectrum, principles of EI mass spectrometer. Types of fragments: odd electron and even electron containing neutral and charged species (even electron rule), Nitrogen rule, isotopic peaks, determination of molecular formula, metastable ion peaks. High resolution mass spectrometry. Salient features of fragmentation pattern of organic compounds including β-cleavage, Mclafferty rearrangement, retro Diels – Alder fragmentation and ortho effect. Principle of EI, CI, Fast Atom Bombardment (FAB), Secondary Ion Mass Spectrometry (SIMS), Electrospray (ESI) ionization and Matrix Assisted Laser Desorption Ionization (MALDI) methods. Introduction to principle and applications of Gas Chromatography-Mass Spectrometry (GC-MS) and Liquid Chromatography-Mass Spectrometry (LC-MS) techniques.

ASP-08: Photoelectron & ESR spectroscopy **15h**

Photoelectron Spectroscopy

Principle and Instrumentation, Types of Photoelectron Spectroscopy – UPS & XPS. Binding Energies, Koopman's Theorem, Chemical Shifts. Photoelectron Spectra of Simple Molecules: N_2, O_2, F_2, CO - 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 and quadrupolar interactions.
Study of free radicals and transition metal complexes. Evidence for covalency in complexes, ex. Cu(II) Bissalcylaldimine, Bis-acetylacetanatovanadyl(II) and hexachloroiridium(IV) complexes.

References:

1. Principles of Polarography, Jaroslav Heyrovsky &Jaroslav Kuta, Elsevier, 2013.
2. Principles of Polarography, Kapoor, John Wiley & Sons, 1991.
3. Principles of Instrumental analysis, 7e, Skoog, Holler and Nieman, Harcourt Asia PTE Ltd. 2020
4. Analytical Chemistry-An Introduction, Skoog, West, Holler and Crouch, Saunders College Publishing, 1999.

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6. Principles of Instrumental Analysis, 4e, Skoog and Leary, Saunders College Publishing, 1992.
7. Spectroscopic identification of organic compounds, 8e by R.M. Silverstein and F.X. Webster, John Wiley & Sons, 2014
8. Instrumental Methods of Chemical Analysis by B K Sharma, Krishna Prakashan Pvt. Ltd., 2011.
9. Instrumental Methods of Analysis by Willard, New York, Van Nostrand Reinhold Company, 1974.
10. Organic spectroscopy by William Kemp, Palgrave Macmillan, 2019.
11. NMR-A multinuclear introduction by William Kemp, Springer, 1986.
12. Spectroscopic methods in organic chemistry by D.H. Williams and I. Fleming McGraw-Hill Education, 1995.
13. International series of Monographs, Vol. 53: Photoelectron Spectroscopy, Edited by D. Beckerand D. Betteridge 1972.
14. Structural methods in inorganic chemistry, 2e, E.A.V. Ebsworth, 1991.
15. Spectroscopy of inorganic compounds by Jagadamba Singh, Mrityunjay D Pandey and Jaya Singh, Second edition 2024, New Age International (P) Ltd., Publishers.
16. Introduction to Spectroscopy, 5e, Pavia Lampman Kriz. Cengage learning, 2014.

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Paper CHE 481: Inorganic chemistry Lab course **4 h/week**

I. Preparation of complexes:

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

II. Titrimetric Analysis of two ions in a mixture

4. Estimation of Ca^{2+} & Mg^{2+}
5. Estimation of Ba^{2+} & Ca^{2+}
6. Estimation of Ni^{2+} & Cu^{2+}
7. Estimation of Mg^{2+} & Mn^{2+}

III. Analysis of Two component mixtures

8, 9. Separation of Ag^{+} and Ca^{2+} in a mixture and estimation of Ag^{2+} (gravimetric) and Ca^{2+}(volumetric).

10, 11. Separation of Cu^{2+} and Ni^{2+} in a mixture and estimation of Ni^{2+} (gravimetric) and Cu^{2+} (Volumetric)

12, 13. 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:

14. 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:

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 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 CHE 482: Organic Chemistry Lab course **4 h/ week**

Identification of organic compounds systematic qualitative analysis:

Physical data BP / MP, Ignition test, solubility classification, Extra elements-N, S & Halogens, (Lassagnine sodium fusion test, Beilstein test)

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 **8** following compounds to be studied as unknown covering at least one from each of the solubility classes

1. Glucose
2. Benzoic acid
3. 2-Chloro benzoic Acid
4. 4. Anisic acid
5. p-Nitrobenzoic acid
6. p-Cresol
7. p-Chlorophenol
8. β-Naphthol;
9. o/m/p-Chloroanilines
10. N-Methyl aniline
11. N,N-Dimethylaniline
12. Benzamide
13. Benzaldehyde
14. Anisaldehyde/p-chloro benzaldehyde
15. Acetophenone
16. Benzophenone
17. Ethylbenzoate
18. Nitrobenzene
19. Chlorobenzene
20. Bromobenzene
21. Naphthalene
22. Anthracene

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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Paper CHE 483: Physical Chemistry Lab **4 h /week**

I. Data analysis II: Mean and standard deviation; absolute and relative errors; linear regression; covariance and correlation coefficient.

II.Distribution:

1. Distribution of I_2 between cyclohexane and water
2. Distribution of I_2 between cyclohexane and aq.KI solution - calculation of equilibrium constant.

III. Chemical Kinetics:

3. Stoichiometry of Peroxydisulphate - Iodide reaction
4,5. Peroxydisulphate - Iodide reaction: Comparison of strengths of KI solutions by isolation method

IV. Conductometry:

6. Titration of a mixture of strong and weak acids vs strong base
7. Determination of the hydrolysis constant of aniline hydrochloride
8. Determination of solubility product

V. Potentiometry:

9. Titration of Cl^- vs Ag^+ (precipitation titration)
10. Determination of solubility product of sparingly soluble salt

VI. Polarimetry:

11. Inversion of cane sugar catalyzed by 1N HCl
12. Inversion of cane sugar catalyzed by 2N HCl

V. pH metry:

13. Calibration of a pH meter and preparation of phosphate buffers
14. Titration of strong acid vs strong base
15. Titration of weak acid vs strong base and determination of dissociation constant of WA.

References

1. Senior Practical Physical Chemistry B.D. Khosla, V.C. Garg and A. Khosla; R Chand & Co., 2018.
2. Experimental Physical Chemistry: V. Athawale and P. Mathur, New Age, International 2001..
3. Practical Physical Chemistry: B. Vishwanathan and P.S. Raghavan, Viva Books, 2012.
4. Practical in Physical Chemistry: P.S. Sindhu, Laxmi Publications, 2009.
5. Advanced Practical Physical chemistry: J.B.Yadav, Krishna Prakashan Media, 2016.

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Paper CHE 484: Analytical Chemistry -II & Spectroscopy Lab course **4 h/ week**

I. Applied analysis:

1. Estimation of alkali content in antacid by acid base titration method
2. Estimation of ascorbic acid in vitamin C by iodometry
3. Estimation of available oxygen in hydrogen peroxide by permanganometry
4. Estimation of calcium in milk by complexometry
5. Determination of hardness of water by complexometry.

II. Identification of unknown organic compounds from their IR, UV, ^{1}H NMR and MS:

Analysis of recorded spectra of 6 compounds belonging to

6. Aromatic carboxylic acid
7. Alcohol and Phenols
8. Aldehydes and Ketones
9. Amides
10. Esters
11. Alkenes and alkynes.

III. Instrumental Analysis:

i. Conductometry:

12. Titration of a mixture of strong and weak acids vs weak base

ii. Potentiometry:

13. Titration of Fe^{+2} vs $Cr_2O_7^{2-}$ (redox titration)
14. Fe^{2+} vs Ce^{4+} and calculation of formal redox potential of Fe(II)/Fe(III)
15. Fe^{2+} vs MnO_4^- and calculation of formal redox potential of Fe(II)/Fe(III)

iii. pH metry:

16. Titration of a mixture of strong and weak acids vs strong base

References:

1. Vogel's text book of Quantitative Inorganic Analysis, 6th edition, J.Mendham etal, Pearson education ltd (2002)
2. Advanced practical chemistry, R.Mukhopadhyay & P. Chatterjee, NCBA books (2016)
3. Advanced practical inorganic chemistry, Gurdeep Raj, GOEL publishing house (2015)
4. Advanced experimental Inorganic chemistry, Ayodhya Singh, Campus Books International (2006)
5. Senior Practical Physical Chemistry: B.D. Khosla, V.C. Garg and A. Khosla; R Chand & Co., 2018
6. Advanced Practical Physical chemistry: J.B.Yadav, Krishna Prakashan Media, 2016.
7. Organic structures from spectra, 5e, L. D. Field, S. Sternhell, J. R. Kalman by Wiley-Blackwell 2013.

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