

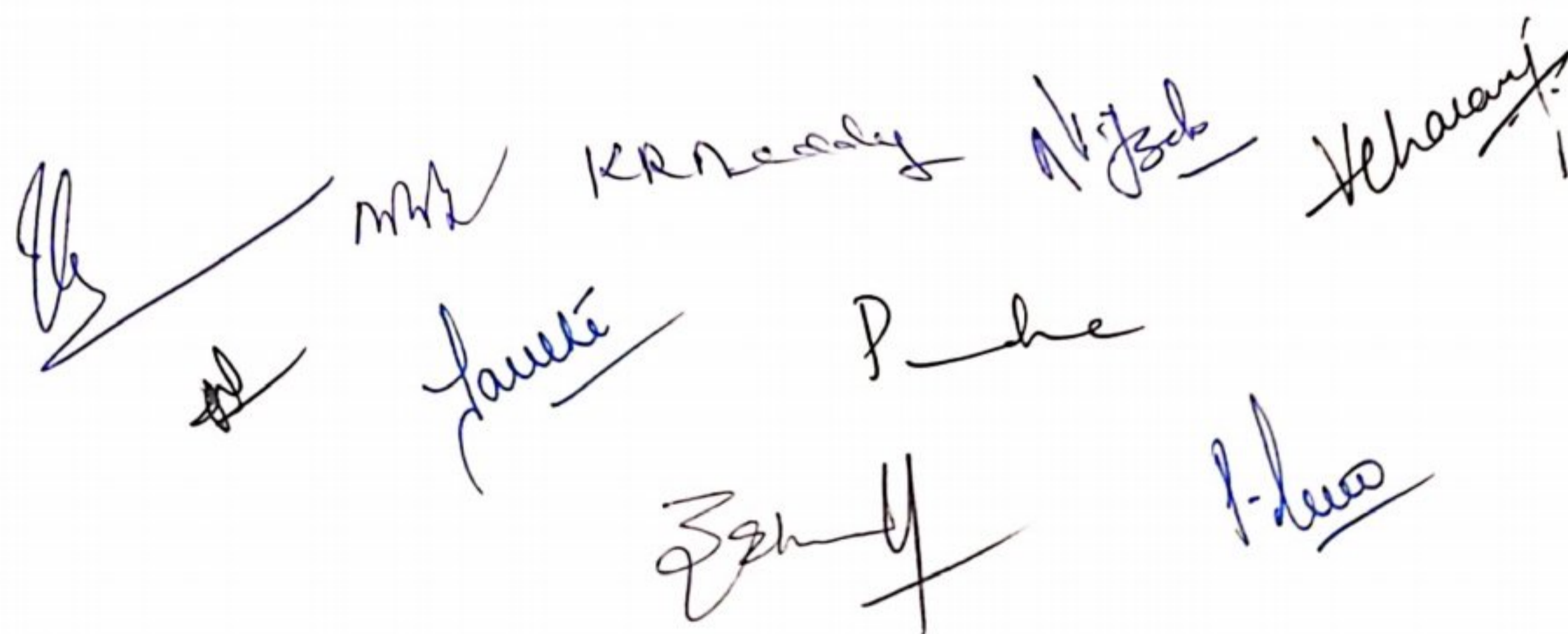
DEPARTMENT OF CHEMISTRY
OSMANIA UNIVERSITY
 (Effective from academic year 2023-2024 for Campus, Constituent and
 Affiliated colleges)

Semester I

	Hrs. /week	internal assessment	Semester exam	Total	Credits
CH101T (*)	3	30 marks	70 marks	100 marks	3
CH102T (*)	3	30 marks	70 marks	100 marks	3
CH103T (*)	3	30 marks	70 marks	100 marks	3
CH104T (*)	3	30 marks	70 marks	100 marks	3
CH151P (IC LAB*)	4			50 marks	2
CH152P (OC LAB*)	4			50 marks	2
CH153P (PC LAB*)	4			50 marks	2
CH154P (AC LAB*)	4			50 marks	2
Total				600 marks	20

Semester II

	Hrs. /week	internal assessment	Semester exam	Total	Credits
CH201T (*)	3	30 marks	70 marks	100 marks	3
CH202T (*)	3	30 marks	70 marks	100 marks	3
CH203T (*)	3	30 marks	70 marks	100 marks	3
CH204T (*)	3	30 marks	70 marks	100 marks	3
CH251P (IC LAB*)	4			50 marks	2
CH252P (OC LAB*)	4			50 marks	2
CH253P (PC LAB*)	4			50 marks	2
CH254P (ACS LAB*)	4			50 marks	2
Total				600 marks	20



M.Sc. CHEMISTRY SYLLABUS

(Effective from academic year 2023-2024 for Campus, Constituent and Affiliated colleges)

SEMESTER -I

Semester-I and Semester-II syllabus is common for all specializations i.e., Inorganic, Organic, Physical, Physical- Organic, Analytical and Pharmacoinformatics.

Paper 1: CH 101 (Inorganic Chemistry)

IC 01: Symmetry of molecules

IC 02: Bonding in Metal Complexes-I

IC 03: Coordination equilibria

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:

15 hrs

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-

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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.

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)

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and 1,1,2,2-tetrahalobutanes.

Conformations of unsaturated acyclic compounds: Propylene, Acetaldehyde and Butanone

Physical methods for conformational Analysis: Use of dipole moment, UV, IR and NMR, spectral methods in conformational analysis.

Conformational affects on the stability and reactivity of acyclic diastereoisomers: Steric and stereoelectronic factors-examples. Conformation and reactivity (E2 eliminations, NGP, Stereochemistry-Rearrangements). The Curtin – Hammett principle.

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. Advanced Organic Chemistry by Jerry March
4. Mechanism and Structure in Organic Chemistry S. Mukerjee
5. Organic chemistry by Jonathan Clayden, Nick Greeves and Stuart Warren
6. Organic Reactions and their mechanisms by P.S. Kalsi
7. Stereochemistry: Conformation & Mechanism by P S Kalsi

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Paper-III: CH 103 (Physical Chemistry)

PC-01: Thermodynamics

PC-02: Electrochemistry

PC-03: Quantum Chemistry-I

PC-01: Thermodynamics

(15 hrs)

Third law of thermodynamics. Evaluation of absolute entropies from heat capacity data for solids, liquids and gases. Standard entropies.

Gibbs equations for non-equilibrium systems. Material equilibrium. Phase equilibrium. Clausius-Clapeyron equation. Conditions for equilibrium in a closed system. The chemical potential. Chemical potential of ideal gases. Ideal-gas reaction equilibrium-derivation of equilibrium constant. Temperature dependence of equilibrium constant-the van't Hoff equation.

Solutions: Partial molar properties-significance. 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. Non ideal solutions. Activities and activity coefficients. Standard-state conventions for non-ideal solutions.

Multicomponent phase equilibrium: Vapour pressure lowering, freezing point depression and boiling point elevation

PC-02: Electrochemistry

(15 hrs)

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 electrodes-Gas electrodes, Metal-metal ion electrodes, reference electrodes, indicator electrode, Ion selective electrodes, Metal-insoluble salt-anion electrodes, Redox electrodes.

Applications of EMF measurements: Solubility product, potentiometric titrations, determination of pH using glass electrode, equilibrium constant measurements. 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's law. Theory of electrolytic conductance. Derivation of Debye-Huckel-Onsager equation – its validity and limitations.

PC-03: Quantum Chemistry- I

(15 hrs)

Wave mechanics and Schrödinger wave equation: Operators- Operator algebra. Commutation of operators, linear operators. Complex functions. Hermitian operators. Operators ∇ and ∇^2 . Eigenfunctions and eigenvalues. Degeneracy. Linear combination of eigenfunctions of an operator. Well behaved functions. Normalized and orthogonal functions.

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M.R. K.R. Reddy
P. d. h.
V. S. S. S. S.
P. S. S. S. S.

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 operatorsignificance. 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 to the spectra of conjugated molecules.

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. Introduction to Electrochemistry, S. Glasstone; East-West Press (Pvt.) Ltd.
6. Modern Electrochemistry, J. O. M. Bockris & A. K. N. Reddy, Plenum
7. Principles of physical chemistry, Samuel H. Maron and Carl F. Prutton, Oxford & IBH
8. Physical Organic Chemistry, N. S. Isaacs, ELBS
09. Elementary Quantum Chemistry, F. L. Pilar, McGraw Hill.
10. Quantum Chemistry – D.A. McQuarrie, Viva Publication
11. Quantum Chemistry, Ira N. Levine, Prentice Hall
12. Introduction to Quantum Chemistry, A.K. Chandra, Tata McGraw Hill
13. Quantum Chemistry, R K Prasad, New Age International Pvt Ltd Publishers

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ES, MS, K Reddy, A Vijaya, H Chandra, P. S. S. S., P. S. S. S., P. S. S. S.

Paper-IV: CH 104 (Analytical Techniques and Spectroscopy – I)

ASP 01: Techniques of Chromatography & Electronic spectroscopy

ASP 02: NMR spectroscopy-I

ASP 03: Vibrational spectroscopy

ASP-01: Techniques of Chromatography and UV Visible Spectroscopy

15 hrs

Techniques of Chromatography: 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 and rate theory.

GC: Principle, instrumentation, detectors - TCD, FID, ECD. Derivatization techniques. Programmed temperature gas chromatography. GC analysis of hydrocarbons in a mixture.

HPLC: Principle, instrumentation, detectors- UV detectors, Photodiode array detector, fluorescence detector. HPLC analysis of paracetamol tablets.

UV Visible Spectroscopy: Principle, selection rules, Woodward-Fieser rules. Congugated dienes, trienes and polyenes. Unsaturated carbonyl compounds, Benzene, mono substituted derivative (Ph-R), di-substituted derivative (R-C₆H₄-R') and substituted benzene derivatives (R-C₆H₄-COR').

ASP 02: NMR spectroscopy-I

15 hrs

¹H NMR spectroscopy: Magnetic properties of nuclei, principles of NMR spectroscopy. Instrumentation: CW and pulsed FT instrumentation. Equivalent and non-equivalent protons. Homotopic, 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, factors affecting coupling constants. Chemically and magnetically equivalent protons.

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(OPEt₃)₄]⁺, [HRh(CN)₅] (Rh I= 1/2).

ASP 03: Vibrational Spectroscopy

15 hrs

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.

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N. Jyotsna
P. S. S.
V. S. S.
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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.

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.

References

1. Fundamentals of Molecular Spectroscopy, Banwell and McCash McGraw Hill
2. Introduction to Molecular Spectroscopy, G.M. Barrow, McGrawHill
3. Absorption Spectroscopy of Organic Compounds, J.R. Dyer Prentice-Hall of India Pvt.Ltd
4. Introduction to Spectroscopy, Pavia Lampman Kriz. Cengage learning
5. Pharmaceutical analysis, Watson Elsevier
6. NMR in Chemistry- A multinuclear introduction, William Kemp, Springer
7. Organic Spectroscopy, William Kemp, Palgrave Macmillan
8. Spectroscopy of organic compounds, P.S. Kalsi, New Age International Publishers
9. Structural methods n Inorganic chemistry, E.A.V Ebsworth, John Wiley & Sons.
10. Organic Spectroscopy, LDS Yadav , Springer
11. Elementary Organic Spectroscopy, Y.R. Sharma S. Chand Limited
12. Molecular Spectroscopy by G Arhuldas, PHI Learning Private Ltd. New Delhi.
13. Vibrational Spectroscopy: Theory and Applications, D. N. Sathyanarayana, New Age International
14. Modern Spectroscopy, J. M. Hollas, John Wiley & Sons

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Practicals

Paper CH 151: Inorganic chemistry Lab course

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)

Paper CH 152: Organic Chemistry Lab course

4 hours/ week

Synthesis of the following compounds:

- 1 p-Bromoacetanilide
- 2 p-Bromoaniline,
- 3 2,4,6- tribromoaniline

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- 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-maleicanhydride adduct
- 12 2,4-Dihydroxyacetophenone
- 13 Phthalimide
- 14 Anthranilic acid
- 15 Methyl-4-nitrobenzoate

References

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

Paper CH 153 Physical Chemistry Lab course

4 hrs / 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.
2. Experimental Physical Chemistry: V. Athawale and P. Mathur, New Age, International.
3. Practical Physical Chemistry: B. Vishwanathan and P.S. Raghavan, Viva Books.
4. Practical in Physical Chemistry: P.S. Sindhu, Laxmi Publications.
5. Advanced Practical Physical chemistry: J.B.Yadav, Krishna Prakashan Media

Paper CH 154: Analytical Chemistry -I Lab course

4 hrs/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
5. Advanced Practical Physical Chemistry: J.B.Yadav

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M.Sc. CHEMISTRY SYLLABUS
(Effective from academic year 2023-2024 for Campus, Constituent and Affiliated colleges)

SEMESTER -II

Semester-I and Semester-II syllabus is common for all specializations i.e., Inorganic, Organic, Physical, Physical- Organic, Analytical and Pharmacoinformatics.

Paper-I: CH 201 (Inorganic chemistry)

IC 04: Reaction mechanisms of transition metal complexes

IC 05: Bonding in metal complexes-II

IC 06: Metal clusters ligational aspects of diatomic molecules

IC-04: 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-05: 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-06: Metal Clusters and Ligational Aspects of Diatomic molecules 15 hrs

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

Metal carbonyl clusters: Bonding modes of CO: Terminal and bridging. 18 Valence electron rule and its applications. Classification of carbonyl clusters. Low nuclearity carbonyl clusters: M₃ and M₄ clusters, structural patterns in M₃(CO)₁₂ (M=Fe, Ru, Os) and M₄(CO)₁₂ (M=Co, Rh, Ir) clusters. High nuclearity carbonyl clusters: M₅, M₆, M₇, M₈ and M₁₀ clusters. Polyhedral skeletal electron pair theory

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Paper-II: CH 202 (Organic Chemistry)

OC-04: Reaction mechanism-II and Molecular Rearrangements,

OC-05: Pericyclic reactions-I

OC-06: Photochemistry

OC-04: Reaction mechanism-II and Molecular Rearrangements

15 hrs

Neighbouring group participation (NGP) : Criteria for determining the participation of neighbouring group. Enhanced reaction rates, retention of configuration, isotopic labeling and cyclic intermediates. NGP involving Halogens, Oxygen, Sulphur, Nitrogen, Aryl. Introduction to nonclassical carbocations; NGP Cycloalkyl groups, σ and π - bonds. (Stereospecific examples of NGP to be covered in conformational analysis)

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

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

OC-05 Pericyclic reactions

15 hrs.

Pericyclic reactions: Introduction, Classification of pericyclic reactions into Electrocyclic, cycloadditions, sigmatropic, ene and chelotropic 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 $4n$ and $4n+2$ cycloadditions.

Sigmatropic reactions: [i, j] 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 -Möbius 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 electrocyclic and cycloadditions & cycloreversions.

OC-06 Organic Photochemistry

15hrs

Photochemistry: Introduction, photochemistry of $\pi-\pi^*$ transitions: Excited states of alkenes, cis-trans isomerisation, and photo stationary state. Photochemistry of 1,3-butadiene, di- π methane

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rearrangement. Intermolecular reactions, photocycloadditions, photodimerisation of simple and conjugated olefins. Addition of olefins to α , β -unsaturated carbonyl compounds. Excited states of aromatic compounds, Photoisomerisation of benzene.

Photochemistry of ($n-\pi^*$) 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 solvent, nature of hydrogen donor and structure of the substrate. Intramolecular abstraction of hydrogen: Norrish type II reactions in ketones, esters and 1,2diketones, Addition to carbon-carbon multiple bonds, Paterno-Buchi reaction, Photochemistry of nitrites: Barton reaction.

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. Maya Shankar Singh, Reactive Intermediates in Organic Chemistry-Structure, mechanism and reactions, Wiley-VCH, 2012.
9. Organic chemistry Vol.I and II by I.L.Finar
10. Comprehensive organic chemistry Vol.5 D.H.R.Barton and W.D..Ollis
11. Pericyclic Reactions - A Textbook: Reactions, Applications and Theory by S. Sankararaman
12. Pericyclic reactions by Ian Fleming.
13. Organic photochemistry by J. M. Coxon and B, Halton
14. Introduction to organic Photochemistry by J. D. Coyle
15. Modern Molecular Photochemistry of Organic Molecules by N J Turro, V. Ramaswamy and J C Scaiano

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Paper-III: CH 203 (Physical Chemistry)

PC-04: Chemical Kinetics and Photochemistry

PC-05: Quantum Chemistry-II

PC-06: Solid State Chemistry:

PC-04: Chemical Kinetics & Photochemistry

(15 hrs)

Chemical Kinetics: Theories of reaction rates: Collision theory, steric factor. Transition state theory. Hammond's postulate. 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- H_2-Br_2 reaction. Derivation of rate law.

Effect of structure on reactivity-Linear free energy relationships. Hammett and Taft equations-substituent (σ and σ^*) and reaction constant (ρ and ρ^*) with examples. Deviations from Hammett correlations, reasons- Change of mechanism, resonance interaction. Taft four parameter equation.

Photochemistry: The Franck Condon principle. Electronically excited molecules- singlet and triplet states. Radiative life times of excited states-theoretical treatment. Measured life times. Quantum yield. Derivation of fluorescence and phosphorescence quantum yields.

Photophysical processes- photophysical kinetics of unimolecular reactions. Calculation of rate constants of various photophysical processes-problems. Photosensitization. Quenching-Stern-Volmer equation. Introduction to fast reactions- Principle of flash photolysis.

PC-05: Quantum chemistry-II

(15 Hrs)

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 pots and boundary diagrams.

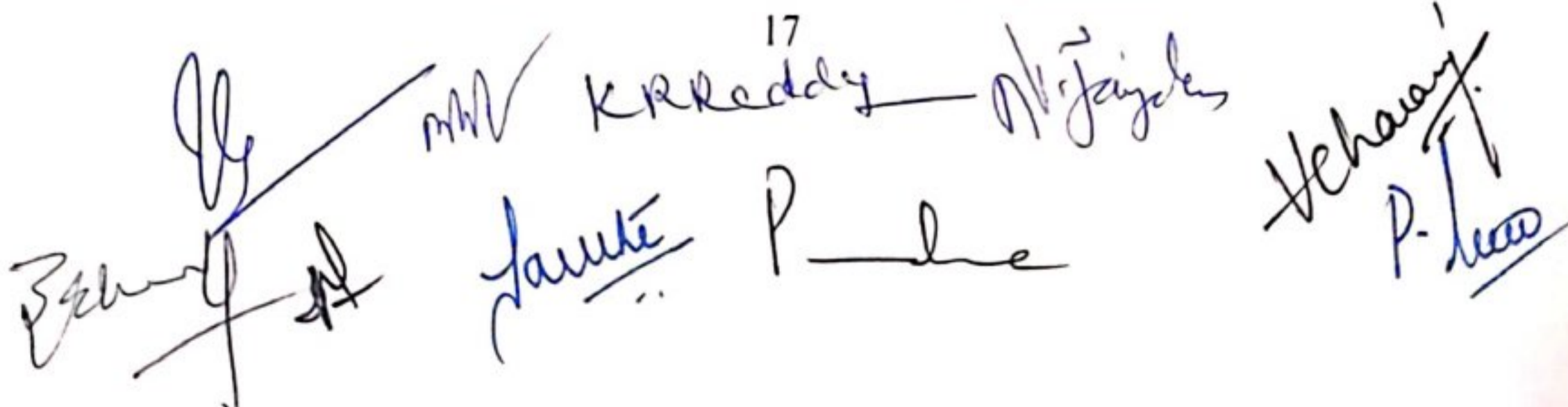
Many electron systems: Approximate methods. The variation method-variation theorem and its proof. Trial variation function and variation integral. Examples of variational calculations. Particle in a box. Construction of trial function by the method of linear combinations. Variation parameters. Secular equations and secular determinant.

Bonding in molecules: Molecular orbital theory-basic ideas. Construction of MOs by LCAO, H_2^+ ion. The variation integral for H_2^+ 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 wave function and the energy of H_2 molecule MO by LCAO method and Valence bond method (detailed calculations not required)-comparison of MO and VB models.

PC-06: Solid state chemistry

(15 Hrs)

Electronic properties of metals, insulators and semi-conductors: Electronic structure of solids, Band theory, Fermi level, K space and Brillouin Zones, 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 $YBa_2Cu_3O_{7-x}$. 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, chemical vapour deposition method and thermolysis. Characterization of nanoparticles – experimental methods – Powder X-ray Diffraction, Scanning electron microscope (SEM), Transmission Electron Microscopy (TEM), and Atomic Force Microscopy (AFM) (Instrumentation not required). Optical properties of nanoparticles, Applications of nanoparticles.

References

1. Physical Chemistry-A Molecular approach, D.A. McQuarrie and J.D. Simon, Viva Books Pvt Ltd
2. Elements of Physical Chemistry by Peter Atkins and Julio de Paula, Oxford University Press
3. Chemical Kinetics and Reaction Mechanisms, J. H. Espenson, McGraw Hill
4. Chemical Kinetics, K.J. Laidler, McGraw Hill
5. The Physical Basis of Org. Chemistry by Howard Maskill, Oxford Univ. Press (New York)
6. Fundamentals of Photochemistry, K.K. Rohtagi-Mukherji, Wiley-Eastern
7. Molecular Reactions and Photo chemistry by Depuy and Chapman
8. Molecular Photochemistry, N.J. Turro, Benjamin
9. Photochemistry, R.P. Kundall and A. Gilbert, Thomson Nelson
10. Essentials of Molecular Photochemistry by A. Gilbert and J. Baggott, Blackwell Scientific Publications.
11. Organic Photochemistry by J.M. Coxon and B. Halton, Cambridge University press.
12. Introductory Photochemistry by A. Cox and T.J. Kemp. McGraw-Hill, London.
13. Quantum Chemistry, D.A. McQuarrie, Prentice Hall
14. Quantum Chemistry, Ira N. Levine, Prentice Hall
15. Introduction to Quantum Chemistry, A.K. Chandra, Tata McGraw Hill
16. Quantum Chemistry, R K Prasad, New Age International Pvt Ltd Publishers
17. Elementary Quantum Chemistry, F. L. Pilar, McGraw Hill.
18. Introduction to Solids, Leonid V. Azaroff, Tata McGraw Hill
19. Solid state Chemistry, D.K. Chakrabarty, New Age International
20. Solid state Chemistry and its applications, A.R. West, Plenum.
21. Principles of the Solid State, H. V. Keer, New Age International
22. The physics and chemistry of solids by Stephen Elliott, Wiley Publishers.
23. Nanostructured Materials and Nanotechnology, edited by Hari Singh Nalwa, Acad. Press
24. Self-Assembled Nanostructures, Jin Zhang, Zhong-lin Wang, Jun Liu, Shaowei Chen & Gan-Yu-Liu, Kluwer Academic/Plenum
25. Introduction to Nanotechnology, Charles P. Poole Jr, F. J. Owens, Wiley India Pvt. Ltd.

Paper-IV: CH 204 (Analytical Techniques and Spectroscopy – II)

15 hrs

ASP 04: Electro and Thermal Analytical Techniques

ASP 05: NMR-II and ESR Spectroscopy

ASP 06: Mass spectrometry

ASP- 04: Electro and Thermal Analytical Techniques

Electro analytical techniques: Types and Classification of Electro analytical Methods.

Polarography: Types of polarography: A.C Polarography and D.C Polarography. D.C Polarography: Instrumentation - Dropping mercury electrode, polarogram. Types of Currents: Residual, Migration and Limiting currents. Two and Three electrode assemblies. Ilkovic equation (derivation not necessary) and its consequences. Applications of polarography in qualitative and quantitative analysis. Analysis of mixtures. Application to inorganic and organic compounds. Determination of stability constants of complexes.

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.

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

Thermal Analysis:

Introduction, types of thermo analytical methods.

Thermogravimetry: Principle and applications of thermogravimetry- Study of calcium oxalate, calcium sulphate and silver nitrate, Differential thermal analysis: Principle and applications of DTA- Differential thermogram of sulphur,

Differential scanning calorimetry DSC: Principle and application of DSC- determination of glass transition temperatures and heat capacities of PVC and Bakelite.

ASP- 05: NMR-II and ESR Spectroscopy

15 hrs

Multinuclear NMR (^1H , ^{19}F and ^{31}P NMR) 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 , H_3PO_4 , H_3PO_3 , H_3PO_2 , HPF_2 , PF_6^- , PH_3 , $[\text{Rh}(\text{PPh}_3)_3\text{Cl}]$ (Rh: I = $\frac{1}{2}$).

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

Electron Spin Resonance Spectroscopy: Introduction, principle, instrumentation, selection rules, calculation of 'g'. Study of free radicals.

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ASP - 06: Mass spectrometry

15 hrs

Origin of mass spectrum, principle 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, Atmospheric Pressure Ionisation (API), Secondary Ion Mass Spectrometry (SIMS), Electrospray ionization (ESI) and Matrix Assisted Laser Desorption Ionization (MALDI) methods.

Introduction, principle and applications of Gas Chromatography-Mass Spectrometry (GC-MS) and Liquid chromatography-Mass Spectrometry (LC-MS) techniques.

References:

1. Principles of Polarography, Heyrovsky, Elsevier Inc.
2. Principles of Polarography, Kapoor, John Wiley & Sons.
3. Modern Electroanalytical methods, edited by C.C harlot, Elsevier Company.
4. Principles of Instrumental analysis, Skoog, Holler and Nieman, Harcourt Asia PTE Ltd.
5. Analytical Chemistry-An Introduction, Skoog, West, Holler and Crouch, Saunders College Publishing.
6. Principles of Instrumental Analysis, Skoog and Leary, Saunders College Publishing.
7. Spectroscopic identification of organic compounds by R.M. Silverstein and F.X. Webster, John Wiley & Sons
8. Instrumental Methods of Chemical Analysis by B K Sharma, Krishna Prakashan Pvt. Ltd.
9. Instrumental Methods of Analysis by Willard, New York, Van Nostrand
10. Organic spectroscopy by William Kemp, Palgrave Macmillan.
11. NMR-A multinuclear introduction by William Kemp, Springer
12. Spectroscopic methods in organic chemistry by D.H. Williams and I. Fleming McGraw-Hill Education

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Practicals

Paper CH 251: Inorganic chemistry Lab course

4 hours/ 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 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^{2+} (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 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)

Paper CH 252: Organic Chemistry Lab course

4 hours/ week

Identification of organic compounds systematic qualitative analysis:

1. BP / MP, Ignition test, solubility classification
2. Extra elements-N,S & Halogens,(Lassaigne sodium fusion test)
3. p-Nitrobenzoic acid/2-Chloro benzoic Acid

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A. Jaiswal, M.M. K. R. S. P. Ch. A. Jaiswal, H. Chaurasiya, P. Ch. P. Ch. P. Ch.

4. Anisole
5. p- Chlorophenol
6. p-Chloroanilines
7. N-Methyl aniline/N-Ethylaniline
8. N,N-Dimethylaniline
9. Benzamide
10. p-Chloro benzaldehyde
11. Acetophenone/ P-Chloro acetophenone,
12. Benzophenone
13. Nitrobenzene
14. Ethylbenzoate
15. Chlorobenzene/ Bromobenzene

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

Paper CH 253: Physical Chemistry Lab

4hrs /week

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

II. Distribution:

1. Distribution of I₂ between cyclohexane and water
2. Distribution of I₂ 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 weak acid

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References

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

Paper CH 254: Analytical Chemistry -II & Spectroscopy Lab course

4 hours/ 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. Spectral analysis: Interpretation of IR, UV, ¹H NMR and MS of the following representative compounds

6. An aldehyde
7. An alcohol
8. A carboxylic acid
9. An amine
10. A Ketone

III. Instrumental Analysis:

Conductometry:

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

Potentiometry:

12. Titration of Fe²⁺ vs Cr₂O₇²⁻ (redox titration)
13. Fe²⁺ vs Ce⁴⁺ and calculation of formal redox potential of Fe(II)/Fe(III)
14. Fe²⁺ vs MnO₄⁻ and calculation of formal redox potential of Fe(II)/Fe(III)

pH metry:

15. 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
6. Advanced Practical Physical Chemistry: J.B.Yadav
7. Organic structures from spectra: L. D. Field, S. Sternhell, J. R. Kalman.

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