DEPARTMENT OF CHEMISTRY SATAVAHANA UNIVERSITY - KARIMNAGAR

REVISED SYLLABUS

From 2022-23 onwards

M.Sc. Chemistry

1& 11 Semester



2023

DEPARTMENT OF CHEMISTRYSATAVAHANA UNIVERSITY - KARIMNAGAR

M.Sc. Chemistry
Under Choice Based Credit System (CBCS)
(From the academic year 2022-23)

M.Sc. (CHE) I SEMESTER

Paper Code	Title	Workload Per Week		Marks			Credits	Duratio n of the
Couc		Theory	Practical	Internal	University	Total		Exams.
MCHE 101T	Inorganic Chemistry-I	4	10 = 3	20	80	100	4	3 Hrs
MCHE 102T	Organic Chemistry-I	4		20	80	100	4	3 Hrs
MCHE 103T	Physical Chemistry-I	4	- 10 <u>- 1</u> 0 (13)	20	80	100	4	3 Hrs
MCHE 104T	Analytical Techniques & Spectroscopy -I	4	14 = 12	20	80	100	4	3 Hrs
MCHE 105P	MCHE Inorganic Chamistry I AP I		6	-	75	75	3	4 Hrs
MCHE 106P	Organic Chemistry LAB-I	-	6	-	75	75	3	4 Hrs
MCHE 107P	Physical Chemistry LAB-I		6	-	75	75	3	4 Hrs
	TOTAL	16	18	80	545	625	25	

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COURSE NAME	M.Sc.	SUBJE	ECT NAME	CHEMISTRY	Max. Marks	80+20
Semester	I	TITLE	INORGANI	C CHEMISTRY-I	No. of Credits	4

Paper-I MCHE 101T: Inorganic Chemistry-I

4 Hrs/ Week

	Taper-Twichte Torr. Inorganic Charles
1	IC-01: Symmetry of molecules
	IC-02: Bonding in Metal Complexes-I
	IC-03: Coordination equilibria
THE STREET, STREET,	IC-04: Ligational aspects of diatomic molecules

IC-01: Symmetry of Molecules

(15Hrs)

Concept of Symmetry in Chemistry – Symmetry Operations – 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 – More about Symmetry Elements – Molecular Point Groups: Definition and Notation of Point Groups, Classification of Molecules in to 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, T_h , T_d , O, O_h , I, I_h , K_h Groups. Descent in Symmetry with Substitution – Exercises in Molecular Point Groups – Symmetry and Dipole moment – Symmetry criteria for Optical activity.

IC-02: Bonding in Metal Complexes- I

(15Hrs)

Crystal Field Theory: Salient features of CFT. d-orbital splitting patterns in regular octahedral, tetragonally distorted octahedral, Jahn-Tellar theorem- tetrahedral, square planar, trigonal planar, and linear geometries. Factors influencing the magnitude of crystal field splitting in octahedral complexes nature of metal ions, nature of ligands, geometry. Concept of weak field and strong fields - Calculation of crystal field stabilization energies (CFSE's) in six and four coordinate 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 Gouy's method. Applications of magnetic moment data for the determination of oxidation states, bond type and stereochemistry. Spin crossover:

IC-03: Coordination Equilibria

(15Hrs)

Salvation of metal ions - Binary complexes: Formation of binary Metal Complexes and their stability – types of Stability Constants – relation between them- trends in Step-wise Stability Constants (Factors causing decrease and increase in Step-wise Stability) – Factors influencing the stability constants: (i) Ligand effects: Basicity, Substituent, Steric, Chelate (size and number of chelate rings), Macro cyclic and Cryptate effects- (ii) Metal ion effects: Ionic potential, Effective Nuclear charge and Atomic Number (Irving-William's Order, geometry of Metal ion and Ligand) – Chelate effect and its Thermodynamic origin – Jahn-Tellar effect on Stability constants of Metal complexes – Pearson's Theory of Hard and Soft Acids and Bases (HSAB), Applications of HSAB, Electronegativity Vs Hardness and Softness. Symbiosis – Methods used for the determination of Stability constants (Basic Principles only): 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 Mo(0) dinitrogen complexes; Chemical fixation of dinitrogen.

References:

- 1. Symmetry and Group theory in Chemistry, Mark Ladd, Marwood Publishers, London (2000).
- 2. Molecular Symmetry and Group Theory, Robert L.Carter, John Wiley & Son (1998).
- 3. Symmetry and Spectroscopy of Molecules. K. Veera Reddy, New Age International (P) Limited (1999).
- Advanced Inorganic Chemistry. F.A.Cotton, G.Wilkinson, C.A.Murillo and M.Bochmann, 6th Edition, Wiley Interscience, N.Y (1999)
- 5. Inorganic Chemistry, J.E.Huheey, K.A.Keiter and R.L.Keiter 4th Edition Harper Cottens College Publications (1993).
- 6. Homogeneous Catalysis by Metal complexes Vol I, M M Taqui Khan and A E Martell, Academic Press NY (1974).
- 7. Inorganic Chemistry, Keith F.Purcell and John C.Kotz, Holt-Saunders International Editions, London (1977).

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COURSE NAME	M.Sc.	SUBJECT	NAME	CHEMISTRY	Max. Marks	80+20
Semester	I	TITLE	ORGAN	NIC CHEMISTRY-I	No. of Credits	4

Paper-II MCHE 102T: Organic Chemistry-I

4 Hrs/ Week

Tap	er-in with 1021. Organic Chemistry
OC-	01: Stereo Chemistry
OC-	02: Reaction Mechanism
OC-	03: Molecular Rearrangements
OC-	-04: Heterocyclics and Natural Products

OC-01: Stereo Chemistry

(15Hrs)

Molecular representations: Wedge, Fischer, Newmann, Sawhorse formulae, their description and inter conversions. Molecular symmetry and chirality: symmetry operations, symmetry elements and criteria of chirality. Configurational nomenclature: Axially chiral allenes, spiranes, alkylidene cycloalkanes. Planar chiral ansa compounds and trans cyclooctene. Determination of configuration: R, S configuration of organic molecules, E, Z nomenclature for unsaturated compounds. Determination of configuration of E, Z isomers by spectral and chemical methods. Determination of configuration of aldoximes and ketoximes. Re, Si faces, Prochirality, Racemization and racemic modifications, Resolution techniques. Principles of chemical reactivity: Kinetic control and thermodynamic control. Introduction to stereo selective synthesis. Concept of dynamic enantiomerism. Atropisomerism.

OC-02: Reaction Mechanism

(15Hrs)

Nucleophilic aromatic substitution: Aromatic nucleophilic substitution S_N1 (Ar), S_N2 (Ar) and benzyne mechanisms.

Neighboring group participation: Enhanced reaction rates, retention of configuration. Neighbouring group participation involving Halogens, oxygen, nitrogen, aryl groups, σ and π bonds. Introduction to non classical carbocations.

Elimination reactions: Elimination reactions E2, E1, E1cB mechanism, orientation and stereo chemistry of E2 elimination, Pyrolytic Syn elimination, elimination Vs Substitution.

Investigation of reaction mechanisms: Kinetics, study of Intermediates, Use of isotopes and Product analysis. Chemical trapping, cross over experiments.

OC-03: Molecular Rearrangements

(15Hrs)

- 1) Generation, stability and reactivity of Carbonium ions, Carbanions, Nitrenes, Free-radicals and Benzynes.
- 2) Molecular rearrangements involving electron deficient carbon: Wagner-Merwein rearrangement, Pinacol-pinacolone rearrangement.
- 3) *Molecular rearrangements involving electron deficient nitrogen:* Hoffman, Curtius, Beckmann rearrangements.
- 4) *Molecular rearrangements involving electron deficient oxygen:* Baeyer villiger oxidation. Base catalysed rearrangements favorski rearrangement, Benzilic acid, Fries rearrangements

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OC-04: Heterocyclics and Natural Products

(15Hrs)

Heterocyclics: Importance of Heterocyclic compounds. Introduction, Nomenclature, synthesis and reactivity of Indole, Quinoline, Isoquinoline, Coumarin, Benzofuran, Carbazole, Acridine.

Natural Products: Importance of Natural products as drugs.

Terpenoids: Definition and classification, general methods used in structure determination of terpenes. Isoprene rule and special isoprene rule. Structure determination and synthesis of α -Terpineol and Camphor.

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. Mukherjee
- 5. Guide Book to mechanism in Organic Chemistry, 6th Edition, Peter Sykes
- 6. Reactive intermediates by C.J. Moodey & G.H. Whitham
- 7. Organic chemistry-volume-I & II by I. L. Finar
- 8. Organic Chemistry by Morrison and RN Boyd
- 9. Heterocyclic chemistry by Raj K. Bansal
- 10. Heterocyclic chemistry by Joule and Smith
- 11. Terpenoids by Mayo

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COURSE NAME	M.Sc.	SUBJECT	NAME	CHEMISTRY	Max. Marks	80+20
Semester	I	TITLE	PHYSI	CAL CHEMISTRY-I	No. of Credits	4

Paper II MCHE 103T: Physical Chemistry-I

4 Hrs/ Week

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PC-01: Thermodynamics-I	artie fulfiller
PC-02: Electrochemistry-I	
PC-03: Quantum Chemistry-I	sementaries
PC-04: Chemical Kinetics-I	

PC-01: Thermodynamics-I

(15Hrs)

Mathematical preliminaries — Derivatives of a function and principles of differentiation (sum, difference, product, quotient, exponential, logarithmic, trigonometric and combined functions), partial differentiation, integral of a function and definite integrals.

Brief review of concepts of I and II laws of thermodynamics. Concept of Entropy, Entropy as a function of V and T, Entropy as a function of P and T. Entropy change as criterion for spontaneity and equilibrium. Third law of thermodynamics. Evaluation of absolute entropies from heat capacity data for solids, liquids and gases. Standard entropies and entropy changes of chemical reactions. Thermodynamic relations. Gibbs equations Gibbs Helmholtz equation. Maxwell relations. Gibbs equations for non- equilibrium systems. Material equilibrium. Phase equilibrium. Clapeyron equation and Clausius-Clapeyron equation. Numerical problems. Conditions for equilibrium in a closed system. Ideal-gas reaction equilibrium-derivation of equilibrium constant. Temperature dependence of equilibrium constant-the Van't Hoff equation.

PC-02: Electrochemistry- I

(15Hrs)

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. Applications of EMF measurements and numerical problems: 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 law. Theory of electrolytic conductance. Derivation of Debye-Huckel-Onsager equation — its validity and limitations.

PC-03: Quantum Chemistry- I

(15Hrs)

A brief review of Black body radiation-Plank's concept of quantization- Plank's equation, average energy of oscillator (derivation not required), wave particle duality and uncertain principle-significance of these for microscopic entities. Emergence of quantum mechanics. Wave mechanics of Schrödinger wave equation. Operators- Operator algebra. Commutation of operators, linear operators. Complex functions. Hermitian operators. ∇ and ∇^2 Operators. Eigen functions and Eigen values. Degeneracy. Linear

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combination of Eigen functions of an operator. Well behaved functions. 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 Eigen values. Eigen functions of commuting operators-significance. Simultaneous measurement of properties and the uncertainty principle. Particle in a box- one dimensional and three dimensional. Energy and wave function. Degeneracy of energy levels. Application to the spectra of conjugated molecules.

PC-04: Chemical Kinetics- I

(15Hrs)

Theories of reaction rates: Collision theory, steric factor. Limitation and numerical problems of Transition state theory. Thermodynamic formulation of transition state theory. Potential energy surface diagram, Reaction coordinate, Activated complex, Activation parameters and their significance. The Eyring equation. Numerical problems. Uni molecular reactions and Lindemann's theory. Numerical problems 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 deviation from Hammett's correlations –reasons – change of mechanism and resonance interactions. Taft equations-substituent constant (σ and σ *) and reaction constant (ρ and ρ *) with examples. Taft four parameter equation. Correlations for Nucleophillic reactions. The Swain — Scott equation and the Edward equation. Reactions in solutions: primary and secondary salt effects

References:

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

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COURSE NAME	M.Sc.	SUBJE	CT NAME CHEMISTRY	Max. Marks	80+20
Semester	I	TITLE	Analytical Techniques & Spectroscopy-I	No. of Credits	4

Paper-IV MCHE 104T: Analytical Techniques & Spectroscopy -I

4 Hrs/ Week

ASP 0	1: Chromatography Techniques
	2: Rotational and Vibrational Spectroscopy
ASP 03	3: Raman and Electronic Spectroscopy
ASP 0	4: NMR Spectroscopy-I (¹ H-NMR)

ASP-01: Chromatography Techniques

(15Hrs)

- i. Introduction, Classification of chromatographic techniques, differential migration rates, partition ratio, retention time, relation between partition ratio and retention time, capacity factor, selectivity factor. Efficiency of separation- resolution, diffusion, plate theory and rate theory.
- ii. GC: Principle, instrumentation, detectors- TCD, FID, ECD.
- iii. HPLC: Principle, instrumentation, detectors- UV detectors, Photodiode array detector, fluorescence detector.

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

ASP -02: Rotational and Vibrational Spectroscopy

(15Hrs)

- a) **Principles of Spectroscopy:** Interaction of the electromagnetic radiation with matter, Types of the energies and molecular spectroscopy, Absorption and emission of the radiation.
- b) Microwave Spectroscopy: Classification of molecules based on moment of inertia. Rigid rotator model, energy levels and selection rules of rotational spectra- Calculation of bond lengths of hetero nuclear diatomic molecules. Intensity of spectral lines Boltzmann distribution law degenarcy of energy states. Effect of isotopic substitution. Non-rigid rotator, energy levels and its spectrum.
- c) Vibrational Spectroscopy: Vibrational energy levels of diatomic molecules, Anharmonic Oscillator, selection rules (derivation not required). Fundamental, Overtones, and hot bands, Calculation of force constant of diatomic molecules, Instrumentation, sample techniques, Normal modes of vibrations for linear and non-linear molecules (Stretching, bending, scissoring, rocking, twisting, wagging), Functional group frequencies, factors influencing vibrational frequencies, Fermi resonance, Combined bands, Applications of the Infra Red spectroscopy, structure elucidation of simple organic molecules, cis-trans isomerism and hydrogen bonding.

ASP -03: Raman and Electronic Spectroscopy

(15Hrs)

- a) Raman Spectroscopy: Classical and quantum theories of Raman Effect. Rotational Raman and vibrational Raman spectra, Stokes and anti-Stokes lines. Complementary nature of IR and Raman spectra.
- b) Electronic spectroscopy: Origin of the electronic spectra, Elementary energy levels of molecules-selection rules for electronic spectra; types of electronic transitions in molecules. Chromophores: Conjugated dienes, trienes and polyenes, unsaturated carbonyl compounds, benzene and its derivatives,

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Woodward-Fieser rules. Polynuclear aromatic hydrocarbons and diketones. Solvent and structural influences on absorption maxima, stereochemical factors. Cis-trans isomers, and cross conjugation. Beer's law application to mixture analysis and dissociation constant of a weak acid. Charge transfer spectra of complexes, photometric titrations.

ASP -04: NMR Spectroscopy-I (¹H-NMR)

(15Hrs)

Magnetic properties of nuclei, Principles of NMR. Instrumentation, CW and pulsed FT instrumentation, relaxation phenomenon, spin-spin and spin-lattice relaxations, equivalent and non equivalent protons, Chemical shift, factors affecting the chemical shift, electro negativity and anisotropy, shielding and deshielding effects, Signal integration, Spin-spin coupling, Coupling constants and factors affecting coupling constants. NMR spectra of ethyl alcohol, vinyl chloride and mono-substituted benzenes (anisole, benzaldehyde and ethyl benzene). Applications of ¹H-NMR spectroscopy: hydrogen bonding, proton exchange processes (alcohols, amines and carboxylic acids), deuterium exchange reactions. First order and non-first order spectra e.g., AX, AX₂, AB, ABC, ABX, and AMX. NOE and its applications, lanthanide shift reagents.

References:

- 1. Fundamentals of Molecular Spectroscopy, Banwell and McCash.
- 2. Molecular Structure and Spectroscopy, G. Aruldas
- 3. Introduction to Molecular Spectroscopy, G.M. Barrow.
- 4. Introduction to Spectroscopy, Pavia, Lampman, Kriz and Vyvyan.
- 5. Absorption Spectroscopy of Organic Compounds, J.R. Dyer.
- 6. Biochemistry: Hames and Hooper.
- 7. Pharmaceutical analysis, Watson
- 8. NMR in Chemistry- A multinuclear introduction, William Kemp.
- 9. Organic Spectroscopy, William Kemp.
- 10. Nuclear Magnetic Resonance basic Principles by Atta-ur-Rahman
- 11. Organic Spectroscopy: Principles and Applications by Jag Mohan
- 12. Spectroscopy of organic compounds, P.S. Kalsi.
- 13. Structural methods n Inorganic chemistry, E.A.V Ebsworth.
- 14. Basic Principles of Spectroscopy, Raymond Chang.

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COURSE NAME	M.Sc.	SUBJEC	T NAME	CHEMISTRY	Max. Marks	75
Semester	I	TITLE	INORGA	NIC CHEMISTRY LAB-I	No. of Credits	3

Paper-V MCHE 105P: Inorganic Chemistry Lab-I

6 hrs/week

1. Calibrations

- a) Calibration of weights
- b) Calibration of Standard flask
- c) Calibration of Burette
- d) Calibration of Pippets

2. Preparation of Complexes

- a) Hg[Co(SCN)₄]
- b) [Cu(NH₃)₄]SO₄
- c) $K_3[Fe(C_2O_4)_3]$
- d) [Mn(acac)₃]
- e) [Ni (en)₃S₂O₃]
- f) [Co(NH₃) ₅Cl]Cl₂

3. Titration Methods with EDTA

- a) Back Titration of i) Ni ⁺² and ii) Al ⁺³ b) Substitution Titration of Ca ⁺²

4. Water Analysis

a) Determination of Total, Permanent and Temporary Hardness of Water

References:

- 1. Text book of Quantitative Inorganic Analysis by A.I.Vogel, 3rd edition, ELBS 1969.
- 2. Vogel's text book of Quantitative Inorganic analysis. Jeffery etal, 4th edition, ELBS 1988.
- 3. Vogel's text book of Quantitative Inorganic Analysis. 6th edition, Pearson education Ltd. 2002.
- 4. Practical Inorganic chemistry By G.Marr and R.W.Rockett 1972.
- 5. Experimental Inorganic/Physical Chemistry An Investigative integrated approach to Practical Project work. By Mounir A.Malati, 1999.
- 6. Advanced experimental Inorganic chemistry by. Ayodhya Singh.
- 7. Practical Inorganic Chemistry by G.Pass & H. Sutchiffe, 2nd Edition John Wiley & Sons.

MODEL QUESTION PAPER

- 1. Preparation of complex
- 2. Determine the Total, Permanent and Temporary hardness of water

SCHEME OF EVAI	LUATION
Assessment	Marks: 75
Complex Preparation	20
Experiment Principle, Calculations and Result (10+25+5)	40
Samples submission	05
Record &Viva-voce	10

COURSE NAME	M.Sc.	SUBJEC	JECT NAME CHEMISTRY		Max. Marks	75
Semester	1 ,	JITLE	ORGAN	IC CHEMISTRY LAB-I	No. of Credits	3

Paper-VI MCHE 106P: Organic Chemistry Lab-I:

6 hrs/week

I. Synthesis of Organic Compounds (Purification-Recrystallization and Calculation of yield)

1) One step Preparations:

- a) m-dinitro benzene
- b) Tetra hydro carbazole
- c) 7-hydroxy-4-methylcoumarin
- d) 2, 4-di hydroxyacetophenone

2) Two step Preparations:

- a) Preparation of 1,3,5-Tribromo benzene
 - i) Preparation of 2,4,6-Tribromo aniline from Aniline
 - ii) Preparation of 1,3,5-Tribromo benzene from 2,4,6-Tribromo aniline
- b) Preparation of para bromo aniline
 - i) Preparation of para bromo acetanilide from acetanilide
 - ii) Preparation of para bromo aniline from para bromo acetanilide
- c) Preparation of anthranilic acid
 - i) Preparation of pthalimide from pthalic anhydride
 - ii) Preparation of anthranilic acid from pthalimide.

II. Thin layer chromatography:

- 1) Preparation of TLC plates and determination of purity of a given sample, monitoring the progress of chemical reactions.
- 2) Separation of a mixture of ortho and para-nitroanilines using silica gel as adsorbent and ethyl acetate as the solvent.

References:

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

MODEL QUESTION PAPER

- 1) Synthesize the given organic compound, recrystallise and Calculate the yield of product. (35M)
- 2) Separate the given mixture of ortho and para nitro anilines using silica gel as adsorbent and chloroform as the solvent (25M)

SCHEME	OF EVALUATION
Assessment	Marks: 75
Experiment 1	35
Experiment 2	25
Samples submission	05
· Record & Viva-voce	10

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COURSE NAME	M.Sc.	SUBJEC	T NAME	CHEMISTRY	Max. Marks	75
Semester	I	TITLE	PHYSIC	CAL CHEMISTRY LAB-I	No. of Credits	3

Paper-V MCHE 107P: Physical Chemistry Lab-I

6 hrs/week

Physical properties: Data analysis I: Significant figures, Precision and accuracy

1) Distribution:

- a) Distribution of acetic acid between n-butanol and water
- b) Distribution of iodine between cyclohexane and water

2) Chemical kinetics:

- a) Acid-catalyzed hydrolysis of methylacetate
- b) Peroxydisulphate-I reaction (overall order)
- c) Oxidation of iodide ion by hydrogenperoxide-iodine clock reaction

3) Conductometry:

- a) Titration of strong acid vs strong base
- b) Titration of weak acid vs strong base
- c) Determination of cell constant
- d) Determination of dissociation constant of a weak acid

4) Potentiometry:

- a) Titration of strong acid vs strong base
- b) Titration of weak acid vs strong base
- c) Determination of dissociation constant of a weak acid
- d) Determination of single electrode potential

5) Polarimetry:

- a) Determination of specific rotation of sucrose
- b) Acid-catalyzed hydrolysis of sucrose (inversion of sucrose)

6) Adsorption and others:

- a) Verification of Freundlich Adsorption isotherm of acetic acid on activated charcoal and determine the concentration of given Acetic acid solution.
- b) Determination of critical solution temperature of phenol-water system Effect of added electrolyte on the CST of phenol-water system
- 7) Determination of molecular weight of a polymer by viscometry

References:

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

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MODEL QUESTION PAPER

1) Conductometry:

- a) Standardise the given sodium hydroxide solution using 0.1 M HCl.
- b) Find the concentration of given weak acid using above standard NaOH solution.

2) Potentiometry:

- a) Standardise the given NaOH solution using given 0.1M HCl
- b) Find the concentration of given acid using above standardised NaOH solution.

3) Distribution:

a) Find the distribution constant of ACOH by studying the distribution of ACOH between N- Butanol & Water.

4) Kinetics of acid catalysed hydrolysis of methyl acetate:

a) Find the concentration of given HCl by following the hydrolysis of Methyl Acetate in acid medium you are provided with 1M HCl unknown HCl, Methyl Acetate, 0.5 M NaOH

5) Kinetics of persulphate-iodide reaction:

a) Find the concentration of KI following the reaction between potassium persulphate and potassium iodide by isolation method.

6) Adsorption:

a) Verify Freundlich adsorption isotherm by studying acetic acid activated charcoal system. You are provided 0.5M acetic acid, 0.2M NaOH and charcoal.

7) p^H Metry:

a) Calibrate the given p^H meter with a buffer solution of known p^H and hence determine the p^H of the given solution.

8) Polarimetry:

a) Determine the specific rotation of sucrose by using polarimeter.

SCI	HEME OF EVALUATION
Assessment	Marks: 75
Principle and brief procedure	10
Experiment and tabulation	30
Graphs	10
Calculations and results	10 Parties alleve considerate a setting.
Viva –Voce	10 10 10 10 10 10 10 10 10 10 10 10 10 1
Record	05

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DEPARTMENT OF CHEMISTRY

SATAVAHANA UNIVERSITY - KARIMNAGAR

M.Sc. Chemistry

Under Choice Based Credit System (CBCS)

(From the academic year 2022-23)

M.Sc. (CHE) II SEMESTER

Paper	Cantilland of Relief 120	Workloa	Workload Per Week		Marks			Duration of
Code	11116		Practical	Internal	University	Total	Credits	the Exams.
MCHE 201T	Inorganic Chemistry-II	4	- -	20	80	100	4	3 Hrs
MCHE 202T	Organic Chemistry-II	4	-	20	80	100	4	3 Hrs
MCHE 203T	Physical Lhemistry-II		- -	20	80	100	4	3 Hrs
MCHE 204T	Analytical Techniques & Spectroscopy-II	4	-	20	80	100	4	3 Hrs
MCHE 205P	Inorganic Chemistry LAB-II	-	6	•	75	75	3	4 Hrs
MCHE 206P	Organic Chemistry LAB-II		6		75	75	3	4 Hrs
MCHE 207P	Physical Chemistry LAB-II	-	6	•	75	75	3	4 Hrs
	TOTAL	16	18	80	545	625	25	

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COURSE NAME	M.Sc.	SUBJI	ECT NAME	CHEMISTRY	Max. Marks	80+20
Semester	II	TITLE	INORGANI	C CHEMISTRY-II	No. of Credits	4

Paper-I MCHE 201T: Inorganic Chemistry-II

4 Hrs/ Week

IC 05	5: Reaction mechanism of transition metal complexes
	5: Bonding in metal complexes-II
	7: Metal clusters
IC 08	3: Biocoordination chemistry

IC-05: Reaction mechanism of transition metal complexes

(15Hrs)

Ligand substitution reactions: Energy profile of a reaction – Transition state or Activated Complex. Types of substitution reactions (SE, SN, S_N1 , S_N2).

Ligand substitution reactions in octahedral complexes: Aquation or Acid hydrolysis reactions, Factors effecting Acid Hydrolysis, Base Hydrolysis, Conjugate Base Mechanism, Evidences in favour of S_N1cB Mechanism.

Substitution reactions without Breaking Metal-Ligand bond: Anation reaction, Acid catalyzed Aquation reaction.

Ligand Substitution reactions in Square Planar complexes: Mechanism of Substitution in Square-Planar complexes- Trans-effect, Grienberg's Polarization theory and Π - bonding theory – Applications of Transeffect 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

(15Hrs)

Free ion terms and Energy levels: Configurations, Terms, States and Microstates, Formula for the calculation of microstates pⁿ and dⁿ configurations, L-S (Russel-Saunders) coupling scheme – j-j coupling scheme – Determination of terms for various pⁿ and dⁿ 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. Jahn-Tellor theorem and its effects on terms.

IC-07: Metal Clusters

(15Hrs)

Carbonyl clusters: Factors favouring Metal-Metal bonding - Classification of Clusters -

Low Nuclearity 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. Metal carbonyl scrambling –

High Nuclearity 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 $[Os_6(CO)_{18}]^{2-}$, $[Rh_6(CO)_{16}]$, $[Os_7(CO)_{21}]$, $[Rh_7(CO)_{16}]^{3-}$, $[Os_8(CO)_{22}]^{2-}$, $[Os_{10}C(CO)_{24}]^{2-}$ and $[Ni_5(CO)_{12}]^{2-}$.

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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. Boranes, carboranes, STYX Rule. Stereo chemical non-rigidity in $[Rh_4(CO)_{12}]$ and $[Fe_2(Cp)_2(CO)_4]$.

IC-08: Bio coordination chemistry

(15Hrs)

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: Haemoglobin and Myoglobin Geometric, electronic and magnetic aspects of Dioxygen binding, Oxygen adsorption isotherms and cooperativity in Haemoglobin and its physiological significance, Role of globin chain. Hemerythrin and Hemocyanin: Structure of deoxy forms, oxygen binding, Geometric, electronic and magnetic aspects. Comparison of hemerythrin and Hemocyanin with haemoglobin.

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

Vitamin B6 model systems: Forms of vitamin B6 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 and John Burgess, Addison Wesley Longman (1999).
- 2. Metal ions in Reaction Mechanisms. K. Veera Reddy. Golgotia Publications (P) Ltd.
- 3. Mechanisms of Reactions in Transition Metal Sites. Richard A Henderson, Oxford Science Publications, London (1993)
- 4. Inorganic Reaction Mechanisms, F.Basolo and R.G.Pearson, New York (1967).
- 5. Advanced Inorganic Chemistry. F.A.Cotton, G.Wilkinson, C.A.Murillo and M.Bochmann, 6th Edition, Wiley Interscience, N.Y (1999)
- 6. Inorganic Chemistry, J.E.Huheey, K.A.Keiter and R.L.Keiter 4th Edition Harper Cottens College Publications (1993).
- 7. Inorganic Biochemistry Edited by G.L.Eichorn, Volume I Elsevier (1982).
- 8. The Chemistry of Metal Cluster Complexes. D.F.Shriver, H.D.Kaerz and R.D.Adams (Eds), VCH, NY (1990).
- 9. Inorganic Chemistry, Keith F.Purcell and John C.Kotz, Holt-Saunders International Editions, London (1977).
- 10. Bioinorganic Chemistry, I.Bertini, H.B.Gray, S.J.Lippard and S.J.Valentine, Viva Low-Priced Student Edition, New Delhi (1998).
- 11. Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, W.Kain and B.Schwederski, John Wiley and Sons, NY (1999).

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COURSE NAME	M.Sc.	SUBJEC	TNAME	CHEMISTRY	Max. Marks	80+20
Semester	II	TITLE	ORGAN	NIC CHEMISTRY-II	No. of Credits	4

Paper-II MCHE 202T: Organic Chemistry-II

4 Hrs/ Week

raper-11 WICHE 2021: Organic Chen	nistry-11
OC-05: Conformational Analysis	
OC-06: Organo metallic reagents	
OC-07: Photochemistry	
OC-08: Pericyclic reactions	

OC-05: Conformational Analysis

(15Hrs)

Introduction to conformational isomerism, study of conformations of ethane, butane and 1,2-di halo butanes, halo hydrins and vicinal diols. Factors affecting the stability of conformations. Klyne prelog terminology for conformers and torsion angles. Conformations of unsaturated acyclic compounds, use of physical and spectral methods in determining preferred conformations. Conformations relative stability and reactivity of acyclic diastereomers. Steric and stereo electronic factors with examples. Quantitative correlation between conformation and reactivity; winstein-Holness equation, Curtin-Hammett principle. Stereo Chemistry of additions, eliminations, neighbouring group participation & intra molecular rearrangements.

OC-06: Organo metallic reagents

(15Hrs)

I. Preparation and applications of organo metallic reagents in organic synthesis: 1) Organo Magnesium, 2) Organo Lithium and 3) Organo Copper reagents, Organo boranes in C-C bond formation, 4) Organo silicon reagents: reactions involving β-carbocations and α-carbanions, utility of trimethyl silyl halides.

II. Carbonyl methylenation:

- 1. Phosphorous ylide mediated olefination: a) Witting reaction, b) Horner-Wadsworth Emmons reaction
- 2. Titanium-Carbene mediated olefination: a) Tebbe reagent, b) Petasis reagent

OC-07: Photochemistry

(15Hrs)

Overview of thermal and photo chemical excitations of molecules, Franck Condon principle, Jablonsky diagram-fluorescence and phosphorescence.

Carbonyl photo chemistry: α -Cleavage, γ -hydrogen transfer (Norrish Type- I and Type-II cleavage). Photo reduction, Photo cyclo addition (Paterno-Büchi reaction).

Photochemistry of olefins: Cis-trans isomerisation, conjugated olefins. Photo chemistry of arenes. Di- π -methane rearrangement. Barton reaction. Investigation of mechanism of photochemical reaction-detection of intermediates—sensitization and quenching.

OC-08: Pericyclic reactions

(15Hrs)

Orbital representation of molecular orbitals: Bonding, Nonbonding, Antibonding orbitals, symmetry properties of molecules.

Classification of pericyclic reactions: Electrocyclic reactions, Cycloaddition reactions, Sigmatropic reactions & examples.

Aromatic transition state theory: Concept, Woodward-Hoffmann selection rules for electrocyclic reactions, cycloaddition- cycloreversions and sigmatropic reactions based on ATS aromatic transition state (Huckel-Mobius) approach.

Otto Marin Work

Frontier molecular orbital theory: Concept, Woodward- Hoffmann rules for electrocyclic, cycloaddition-cycloreversions and sigmatropic reactions based on FMO approach.

Conservation of molecular orbitals theory: Concept, framing of Woodward-Hoffmann selection rules for electrocyclic, cycloaddition-cycloreversions based on conservation of molecular orbitals approach.

References:

- 1. Stereochemistry of organic compounds Principles and Applications by D. Nasipuri
- 2. Stereochemistry by V M Potapov
- 3. Hand book of Grignard reagents by Gray S Silverman & Philip E Rakija
- 4. Grignard reagents- New developments by Herman G. Richey
- 5. Basic organo metallic Chemistry by B. D Guptha & A J Elias
- 6. Molecular reactions and photochemistry by Depuy and Chapman
- 7. Organic photochemistry by N. J. Turro
- 8. Organic photo chemistry by D Coyle
- 9. Photochemistry and pericyclic reactions by Jagdamba Singh & Jaya Singh
- 10. Organic Reaction mechanisms S. Mukherjee & Singh
- 11. Pericyclic reactions by Mukherjee.
- 12. Conservation of orbital symmetry by wood ward and Hoffmann

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COURSE NAME	M.Sc.	SUBJECT NAME		CHEMISTRY	Max. Marks	80+20
Semester	II	TITLE	PHYS	ICAL CHEMISTRY-II	No. of Credits	4

Paper III MCHE 203T: Physical Chemistry-II

4 Hrs/ Week

Tapel III WICHE 2031: Physical C	nemistry-11
PC-05: Thermodynamics-II	
PC-06: Photochemistry-I	
PC-07: Quantum Chemistry-II	
PC-08: Solid state chemistry	

PC-05: Thermodynamics-II

(15Hrs)

Solutions: Specifying the Solution composition. Partial molar properties-significance. Relation between solution volume and partial molar volume. Measurement of partial molar volumes- slope and intercept methods. The chemical potential. Variation of chemical potential with T and P. Gibbs-Duhem equation-derivation and significance.

Ideal solutions: Thermodynamic properties of ideal solutions. Mixing quantities. Vapour pressure - Raoult's law. Thermodynamic properties of ideally dilute solutions. Vapour pressure- Henry's law. Non ideal systems. Concept of fugacity, fugacity coefficient. Determination of fugacity. Non ideal solutions. Activity and activity coefficients. Standard-state conventions for non ideal solutions. Determination of activity coefficients from vapour pressure measurements. Activity coefficients of nonvolatile solutes using Gibbs- Duhem equation.

PC-06: Photochemistry -I

(15Hrs)

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

PC-07: Quantum chemistry-II

(15Hrs)

Cartesian, Polar and spherical polar coordinates and their interrelations. Schrodinger equation for the hydrogen atom- separation into three equations. Hydrogen like wave functions. Radial and angular functions. Quantum numbers n, l and m and their importance. The radial distribution functions. Hydrogen like orbitals and their representation. Polar plots, contour plots and boundary diagrams. Many electron systems. Approximate methods. The variation method- variation theorem and its proof. Trial variation function and variation integral. Examples of variational calculations. Particle in a box. Construction of trial function by the method of linear combinations. Variation parameters. Secular equations and secular

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Bonding in molecules. Molecular orbital theory-basic ideas. Construction of MOs by LCAO, H_2^+ ion. The variation an 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.

PC-08: Solid state chemistry

(15Hrs)

Electronic properties of metals, insulators and semi-conductors: Electronic structure of solids, Band theory, band structure of metals, insulators and semi-conductors. Electrons, holes and Excitons. The temperature dependence of conductivity of extrinsic semi-conductors. Photo conductivity and photovoltaic effect — p-n junctions. Superconductivity: Occurrence of superconductivity. Destruction of superconductivity by magnetic fields — Meissner effect. Types of superconductors. Theories of superconductivity — BCS theory.

High temperature superconductors: Structure of defect perovskites. High T_c superconductivity in cuprates. Phase diagram of Y-Ba-Cu-O system. Crystal structure of YBa₂Cu₃O_{7-x}. Preparation of 1-2-3 materials. Origin of high T_c superconductivity. Nanoparticles and their applications: Introduction to nanoparticles. Reduced dimensionality in solids – zero dimensional systems, fullerenes, quantum dots. One dimensional systems, carbon nano tubes, preparation of nanoparticles –top down and bottom up methods. Preparation of nanomaterials – sol gel methods, co-precipitation method and CVD method. Applications of nanoparticles.

References:

- 1. Atkin's Physical Chemistry, Peter Atkins and Julio de Paula, Oxford University press
- 2. Physical Chemistry, Ira N. Levine, McGraw Hill
- 3. Physical Chemistry-A Molecular approach, D.A. McQuarrie and J.D. Simon, Viva Books Pvt Ltd
- 4. Molecular Thermodynamics, D.A. McQuarrie and J.D. Simon, University Science Books
- 5. Quantum Chemistry, Ira N. Levine, Prentice Hall
- 6. Introduction to Quantum Chemistry, A.K. Chandra, Tata McGraw Hill
- 7. Introduction to Solids, Leonid V. Azaroff, Tata McGraw Hill
- 8. Solid state Chemistry, D.K. Chakrabarthy, New Age International
- 9. Solid state Chemistry and its aplications, A.R. West, Plenum.
- 10. Fundamentals of Photochemistry, K.K.Rohtagi-Mukherji, Wiley-Eastern
- 11. Molecular Photochemistry, N.J. Turro, Benjamin
- 12. Photochemistry, R.P.Kundall and A. Gilbert, Thomson Nelson
- 13. Essentials of Molecular Photochemistry by A. Gilbert and J. Baggott, Blackwell Scientific Publications.
- 14. Organic Photochemistry by J.M.Coxon and B.Halton, Cambridge University press.
- 15. Introductory Photochemistry by A.Cox and T.J.Kemp. McGraw-Hill, London.
- 16. Principles of the Solid State, H. V. Keer, New Age International
- 17. Elements of Physical Chemistry by Peter Atkins and Julio de Paula, Oxford University Press
- 18. Nanostructured Materials and Nanotechnology, edited by Hari Singh Nalwa, Academic Press
- 19. Introduction to Nanotechnology, Charles P. Poole Jr, F. J. Owens, Wiley India Pvt. Ltd.
- 20. Nanostructured Materials and Nanotechnology, edited by Hari Singh Nalwa, Academic Press

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COURSE NAME	M.Sc.	SUBJI	SUBJECT NAME CHEMISTRY Max. Mark		Iarks	80+20	
Semester	II	TITLE	Analytical Te	chniques & Spectro	scopy-II	No. of Cr	edits 4

Paper-IV MCHE 204T: Analytical Techniques & Spectroscopy -II

4 Hrs/ Week

ASP-05: Electro Analytical Techniques

(15Hrs)

- a) Types and Classification of Electro analytical Methods:
- i) Potentiometry: Types of electrodes, Hydrogen gas, Calomel, Quin hydrone and glass electrodes. Determination of pH. Potentiometric titrations.
- ii) Conductometry: Definition of terms conductivity, specific conductivity, cell constant.
 Mobility of ions, Conductometric titrations.
- b) D.C Polarography: Dropping mercury electrode- Instrumentation- polarogram. Types of Currents: Residual, Migration, Limiting. Two and Three electrode assemblies. Ilkovic equation (derivation not necessary) and its consequences Types of limiting Currents: Adsorption, Diffusion, Kinetic.

Applications of polarography in qualitative and quantitative analysis. Analysis of mixtures. Application to inorganic and organic compounds. Determination of stability constants of complexes.

- c) Brief account of following techniques and their advantages over conventional d.c. Polargraphy:
- (i) A.C.polarography (ii) Square-wave polarography (iii) Pulse polarography (iv) Differential pulse polarography
- d) Amperometric titrations: Principle, Instrumentation. Types and applications of amperometric titrations. Determination of SO_4^{2-} , metal ions viz., Mg^{2+} , Zn^{2+} , Cu^{2+} and other substances.
- e) Cyclic Voltammetry: Principle, instrumentation, reversible and irreversible cyclic voltammograms. Applications. Cyclic voltammetric study of insecticide parathion.

ASP 06: NMR -II

(15Hrs)

- ¹³C NMR spectroscopy: Introduction to ¹³C NMR spectroscopy, types of ¹³C NMR spectra: undecoupled, proton- decoupled, single frequency off-resonance decoupled (SFORD) and selectively decoupled spectra. ¹³C chemical shifts, factors affecting the chemical shifts, chemical shifts of organic compounds. Homonuclear (¹³C-¹³C J) and heteronuclear (¹³C-¹H J, ¹³C-²H J and ¹³C-¹⁹F J) couplings.
- Applications of ¹³C-NMR spectroscopy: Structure determination, stereochemistry and reaction mechanisms in organic molecules. Principle and applications of DEPT method.
- ¹⁹F NMR spectroscopy: ¹⁹F chemical shifts, coupling constants. Applications of ¹⁹F NMR involving coupling with ¹⁹F, ¹H and ³¹P. CH₃CHFBr, BrF₅, SF₄, PF₅, ClF₃, IF₅, HF₂.
- ³¹P NMR spectroscopy: ³¹P chemical shifts, coupling constants. Applications of ³¹P NMR involving coupling with ³¹P, ¹⁹F, ¹H and ¹³C. P₄S₃, P(OCH₃)₃, H₃PO₄, H₃PO₃, H₃PO₂, HPF₂, PF₆, [Rh (PPh₃)Cl₃] Rh *I*=1/2.

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ASP 07: Mass Spectrometry

(15Hrs)

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, *Mc.* lafferty rearrangement, retro Diels–Alder fragmentation and ortho effect. Principle of EI, CI, Fast Atom Bombardment (FAB), Secondary Ion Mass Spectrometry (SIMS), Electro Spray ionization (ESI) 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: Electron Spin Resonance Spectroscopy

(15Hrs)

Introduction, principle, instrumentation, selection rules, interpretation of Lande's factor 'g'. Hyperfine and super hyperfine Coupling. Anisotropy in 'g' values and hyperfine coupling constants. Zero field splitting, Kramer's degeneracy, quadrupolar interactions.

Application of ESR to the study of simple free radicals: methyl (C_3), ethyl (C_2H_5), 1,4-benzosemiquinone and naphthalene anion, amine (NH_2), diphenyl picryl hydrazyl, cyclopentadienyl (C_5H_5), hydroxy methyl(CH_2OH) Radicals.

Study of free radicals and transition metal complexes: Applications of ESR to Metal Complexes - ESR Spectra of d^1 - d^9 Transition Metal Complexes with examples. Interpretation of g in cubic, axial and rhombohedral geometries. Factors affecting g values. Calculation of g values with simple examples. Interpretation of 'g' and 'A' values from ESR spectral data in i) MnF_6^{4-} , ii) CoF_6^{4-} , and CrF_6^{3-} .

References:

- 1. Principles of Polarography, Heyrovsky.
- 2. Principles of Polarography, Kapoor.
- 3. Modern Electro analytical methods, edited by C.Charlot, 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. Prinicples of Instrumental Analysis, Skoog and Leary, Saunders College Publishing.
- 7. International series of Monographs, Vol. **53**: Photoelectron Spectroscopy, Edited by D. Beckerand D. Betteridge 1972.
- 8. Sructural methods in inorganic chemistry, E.A.V. Ebsworth.
- 9. Spectroscopic identification of organic compounds by R.M. Silverstein and F.X. Webster.
- 10. Organic spectroscopy by William Kemp
- 11. Mass Spectrometry for Chemists and biochemists by M. Rose and R.A. W. Johnstone
- 12. Spectroscopic methods in organic chemistry by D.H. Williams and I. Fleming
- 13. Practical Pharmaceutical Chemistry by A. H. Beckett and J.B. Stenlake
- 14. Biological Mass Spectrometry by A.L. Burlingame
- 15. Principles and Practice of Biological Mass Spectrometry by Chhabil Das
- 16. NMR-A multinuclear introduction by William Kemp
- 17. Nuclear Magnetic Resonance basic Principles by Atta-ur-Rahman
- 18. Organic Spectroscopy: Principles and Applications by Jag Mohan
- 19. Stereochemistry of Carbon compounds by Ernest L Eliel / Samuel H. Wilen

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COURSE NAME	M.Sc.	SUBJE	CT NAME	CHEMISTRY	Max. Marks	7.5
Semester	II	TITLE	INORGAN	IC CHEMISTRY LAB-II	No. of Credits	3

Paper-V MCHE 205P: Inorganic Chemistry Lab-II

6 hrs/week

- 1) Estimation
 - a) Calcium in Milk
- 2) One component gravimetric estimations
 - a) Estimation of Zn⁺²
 - b) Estimation of Ba⁺²
- 3) Analysis of Two Component Mixtures
 - a) Determination of Ferri and Ferro cyanide in the mixture
 - b) Separation and determination of Cu⁺² and Ni⁺² in the mixture
- 4) Analysis of Three Component Mixtures

 a) Separation of Ni⁺² and Cu⁺² from Mg⁺² in the given mixture and estimation of Mg⁺² by Gravimetry

 b) Separation of Fe⁺² and Ni⁺² from Zn⁺² in the given mixture and estimation of Zn⁺² by Gravimetry
- 5) Ion Exchange Methods of Analysis
 - a) Determination of Capacity of an Ion Exchange Resin
 - b) Separation of Zinc and Magnesium on an Anion Exchange Resin and Estimation of Mg⁺² and Zn⁺²

References:

- 1. Text book of Quantitative Inorganic Analysis by A.I.Vogel, 3rd edition, ELBS 1969.
- 2. Vogel's text book of Quantitative Inorganic analysis. Jeffery etal, 4th edition, ELBS 1988.
- 3. Vogel's text book of Quantitative Inorganic Analysis. 6th edition, Pearson education Ltd. 2002.
- 4. Practical Inorganic chemistry By G.Marr and R.W.Rockett 1972.
- 5. Experimental Inorganic/Physical Chemistry An Investigative integrated approach to Practical Project work. By Mounir A.Malati, 1999.
- 6. Advanced experimental Inorganic chemistry by. Ayodhya Singh.
- 7. Practical Inorganic Chemistry by G.Pass & H. Sutchiffe, 2nd Edition John Wiley &Sons.

MODEL QUESTION PAPER

- 1. Estimate the amount of Calcium in the given milk sample
- 2. Determine the amount of Ferri and Ferrocyanide in the given mixture

. SCHEME OF EVALUATION				
Assessment	Marks: 75			
Estimations	20 10 10 10 10 10 10 10 10 10 10 10 10 10			
Analysis (Two Component mixture/ Ion exchange method)	45			
[Principle, Experiment and Result (10+30+5)] Record &Viva-voce	10			

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COURSE NAME	M.Sc.	SUBJECT NAME		CHEMISTRY	Max. Marks	75
Semester	II	TITLE	ORGANI	C CHEMISTRY LAB-II	No. of Credits	3

Paper-VI MCHE 206P: Organic Chemistry Lab-II

6 hrs/week

1) Identification of organic compounds, systematic qualitative analysis:

Physical data BP / MP, Ignition test, Lassaignes test – Nitrogen, Sulphur and halogens, solubility classification, Functional group tests, Preparation of crystalline derivatives and determination of their Melting points and reference to literature to identify the compounds.

A minimum of **14** compounds covering different functional groups and solubility pattern. Glucose; benzoic acid, 2-chloro benzoic acid, anisic acid, p-nitrobenzoic acid; p-cresol, p-chlorophenol, β-naphthol; aniline, o/m/p-chloroanilines, N-methylaniline, N-ethylaniline, N,N-dimethylaniline; benzamide, acetanilide; benzaldehyde, anisaldehyde, acetophenone, benzophenone; ethylbenzoate, methylbenzoate; nitrobenzene, chlorobenzene, bromobenzene, naphthalene, biphenyl and anthracene.

2) Spectroscopic identification of organic compounds

Identification of unknown organic compounds by interpretation of IR, UV, ¹H NMR, ¹³C NMR and mass spectral data. A minimum of **15** representative examples should be studied.

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.

MODEL QUESTION PAPER

- 1) Identify the given unknown organic compound by qualitative analysis and prepare two derivatives of it
- 2) Determine the structure of compound by using the given spectral data of UV, IR, ¹H-NMR, ¹³C-NMR and Mass spectral data

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SCHEME OF EVALUATION Assessment Marks: 75			
Experiment 2	25		
Samples submission	05		
Record & Viva-voce	10		

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COURSE NAME	M.Sc.	SUBJECT NAME		CHEMISTRY	Max. Marks	75
Semester	II	TITLE	PHYSICA	L CHEMISTRY LAB-II	No. of Credits	3

Paper-V MCHE 207P: Physical Chemistry Lab-II

6 hrs/week

1) Distribution:

- a) Distribution of I₂ between cyclo hexane and aq. KI solution-calculation of equilibrium constant.
- b) Study of complex formation between ammonia and metal ion

2) Chemical Kinetics

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

3) Conductometry:

- a) Titration of a mixture of strong and weak acids vs strong base
- b) Determination of the hydrolysis constant of aniline hydrochloride
- c) Determination of solubility product of AgCl

4) Potentiometry:

- a) Titration of Fe⁺² vs $(Cr_2O_7)^{-2}$ (redox titration)
- b) Titration of Cl vs Ag+ (precipitation titration)
- c) Determination of solubility product of AgCl

5) Polarimetry:

- a) Determination of specific rotation of glucose and fructose
- b) Enzyme catalysed inversion of sucrose

6) Colorimetry:

a) Verification of Beer's law and calculation of molar extension coefficient using CuSO₄ and KMnO₄ solutions

7) pH metry:

- a) Calibration of a p^H meter and measurement of p^H of different solutions
- b) Preparation of phosphate buffers
- c) Titration of strong acid vs strong base

References:

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

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MODEL QUESTION PAPER

1) Potentiometry:

a) Find the concentration of given Fe²⁺ potentiometrically. You are provided 0.1M FAS and apox. 0.02M K₂Cr₂O₇.

2) Colorometry:

a) Verify Lambert-Beer's Law using KMnO₄ and CuSO₄ solutions. Find the concentrations of given KMnO₄ and CuSO₄ solutions colorimetrically. You are provided 2x10⁻⁴M KMnO₄ and 0.2M CuSO₄ solutions.

3) Distribution:

a) Find the concentration of given KI solution by studying distribution of Iodine between cyclo hexane and aqueous KI. You are provided saturated solution of I₂ in CCl₄ 0.1M KI and 0.05M Hypo.

4) Kinetics:

a) Find the concentration of KI in the reaction between K₂S₂O₈ and KI kinetically.

5) Conductometry:

a) Standardise the given sodium hydroxide solution using 0.1 M HCl solution.

b) Estimate the concentration of given acids in a mixture. (Strong acid and weak acid).

SCHEME OF EVALUATION				
Assessment	Marks: 75			
Principle and brief procedure	10			
Experiment and tabulation	30			
Graphs	10			
Calculations and results	10			
Viva –Voce	10			
Record	05			

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