C. ABDUL HAKEEM COLLEGE (AUTONOMOUS)

(Affiliated to Thiruvalluvar University, Vellore & Re-Accredited by NAAC with 'A' Grade)

MELVISHARAM – 632 509

PG & Research Department of Chemistry

MASTER OF SCIENCE

DEGREE COURSE

M.Sc., CHEMISTRY

UNDER CBCS

(with effect from 2018-2019)

The Course of Study and the Scheme of Examinations

S. NO.	Study Components		Ins. hrs /week	Credit	Title of the Paper	Maximum Marks		
	Course Title							
SEMESTER I						CIA	Uni. Exam	Total
1	MAIN	Paper-1	5	4	Stereochemistry & Substitution Reactions	25	75	100
2	MAIN	Paper-2	5	4	Structural & Coordination Chemistry	25	75	100
3	MAIN	Paper-3	5	4	Physical Chemistry - I	25	75	100
	MAIN PRACTICAL	Paper-1	4	0	Organic Chemistry Practicals - I	-	-	-
	MAIN PRACTICAL	Paper-2	4	0	Inorganic Chemistry Practicals - I	-	-	-
	MAIN PRACTICAL	Paper-3	4	0	Physical Chemistry Practicals - I	-	-	-
4	ELECTIVE	Paper-1	3	3	**(to choose 1 out of 3)** A. **Polymer Chemistry** B. Heterocyclic Chemistry C. Inorganic Photochemistry	25	75	100
			30	**15**		**100**	**300**	**400**

SEMESTER II						CIA	Uni. Exam	Total
5	MAIN	Paper-4	4	3	Organic Reaction Mechanisms	25	75	100
6	MAIN	Paper-5	4	3	Solid State & Nuclear Chemistry	25	75	100
7	MAIN	Paper-6	5	4	Physical Chemistry - II	25	75	100
8	MAIN PRACTICAL	Paper-1	4	5	Organic Chemistry Practicals - I	25	75	100
9	MAIN PRACTICAL	Paper-2	4	5	Inorganic Chemistry Practicals - I	25	75	100
10	MAIN PRACTICAL	Paper-3	4	5	Physical Chemistry Practicals - I	25	75	100
11	**Compulsory Paper**		2	2	**Human Rights**	25	75	100
12	ELECTIVE	Paper-2	3	3	**(to choose 1 out of 3)** A. **Green Chemistry** B. Material Science C. Applied Electrochemistry	25	75	100
			30	**30**		**200**	**600**	**800**
SEMESTER III						**CIA**	**Uni. Exam**	**Total**
13	MAIN	Paper-7	5	4	Organic Spectroscopy & Natural products	25	75	100
14	MAIN	Paper-8	5	4	Organometallics & Coordination Chemistry	25	75	100
15	MAIN	Paper-9	5	4	Physical Chemistry - III	25	75	100
	MAIN PRACTICAL	Paper-4	4	0	Organic Chemistry Practicals - II	-	-	-
	MAIN PRACTICAL	Paper-5	4	0	Inorganic Chemistry Practicals - II	-	-	-
	MAIN PRACTICAL	Paper-6	4	0	Physical Chemistry Practicals - II	-	-	-
16	ELECTIVE	Paper-3	3	3	**(to choose 1 out of 3)** A. **Scientific Research Methodology** B. Physical Organic Chemistry C. Bioorganic And Medicinal Chemistry	25	75	100
			30	**15**		**100**	**300**	**400**

SEMESTER IV						CIA	Uni. Exam	Total
17	MAIN	Paper-10	5	4	Photochemistry & Biorganic Chemistry	25	75	100
18	MAIN	Paper-11	5	4	Inorganic Spectroscopy & Analytical Techniques	25	75	100
19	MAIN	Paper-12	5	4	Physical Chemistry - IV	25	75	100
20	MAIN PRACTICAL	Paper-4	4	5	Organic Chemistry Practicals - II	25	75	100
21	MAIN PRACTICAL	Paper-5	4	5	Inorganic Chemistry Practicals - II	25	75	100
22	MAIN PRACTICAL	Paper-6	4	5	Physical Chemistry Practicals - II	25	75	100
23	ELECTIVE	Paper-4	3	3	**(to choose 1 out of 3)** A. **Environmental Chemistry** B. Bioinorganic Chemistry C. Chemistry of Natural Products	25	75	100
			30	**30**		**175**	**525**	**700**

Subject	Papers	Credit	Total Credits	Marks	Total marks
MAIN	12	4-5	46	100	1200
MAIN PRACTICAL	6	4-5	30	100	600
ELECTIVE	4	3	12	100	400
COMPULSORY PAPER	1	2	2	100	100
Total	**23**	**-**	**90**	**-**	**2300**

SEMESTER - III

PAPER - 7

ORGANIC SPECTROSCOPY & NATURAL PRODUCTS

OBJECTIVES	To understand the concepts of spectral techniques and to apply these techniques for the quantitative and structural analysis of organic compounds. To understand Terpenes, Alkaloids, Heterocycles, Steroids and their importance.
COURSE OUTCOMES	
CO1	To know the principles of spectroscopy. To understand the various concept of UV Visible and IR spectroscopy. To learn their importance in functional groups identification.
CO2	To acquire knowledge about various principle of ^{1}H-NMR and ^{13}C-NMR. To know the spectroscopic techniques of structural determination of organic molecules.
CO3	To know the basic principle of mass spectroscopy. To understand the structural characteristics of organic molecules.
CO4	To know the chemistry of natural products and their classification. To understand the systematic methods of structural elucidation of natural products.
CO5	To know the significance of natural products. To understand the chemistry of heterocyclic, steroids and their synthesis.

UNIT-I: UV AND IR SPECTROSCOPY AND ITS APPLICATIONS

Ultraviolet - Visible spectroscopy - types of electronic transitions - chromophores and auxochromes - factors influencing position and intensity of absorption bands - absorption spectra of dienes, polyenes and unsaturated carbonyl compounds - Woodward - Fieser rules.

IR Spectroscopy - vibrational frequencies and factors affecting them - identification of following functional groups (hydrocarbons, alcohol, aldehyde, ketone, amine, ester and nitro) - intra and inter molecular hydrogen bonding - finger print region - Far IR region - metal ligand stretching vibrations.

UNIT-II: NMR SPECTRA AND ITS APPLICATIONS

Nuclear spin - magnetic moment of a nucleus - nuclear energy levels in the presence of magnetic field relative populations of energy levels - basic principles of NMR experiments - CW and FT NMR - ^{1}H NMR - chemical shift and coupling constant - factors influencing proton chemical shift and vicinal proton - proton coupling constant - ^{1}H NMR spectra of simple organic molecules such as CH_3CH_2Cl, CH_3CHO etc. AB, AX and ABX spin system - spin decoupling - nuclear overhauser effect- chemical exchange- chemical shift reagents.

^{13}C NMR - proton decoupled and off - resonance ^{13}C NMR spectra - factors affecting ^{13}C NMR chemical shift - ^{13}C NMR spectra of simple organic molecules. Problem solving (for molecules with a maximum number of C_{10}). Elementary concept of COSY and NOESY.

UNIT-III: PHYSICAL METHODS OF STRUCTURAL DETERMINATION

Mass Spectroscopy - Principles - measurement techniques - (El, Cl, FD, FAB, SIMS) - presentation of spectral data - molecular ions - isotope ions - fragment ions of odd and even electron types - rearrangement ions - factors affecting cleavage patterns - simple and multicentre fragmentation - McLafferty rearrangement. Mass spectra of hydrocarbons, alcohols, phenols, aldehydes and ketones. ORD, octant rule, cotton effect, axial halo ketone rule and their applications.

UNIT-IV: CHEMISTRY OF NATURAL PRODUCTS - I

Terpenes: Introduction- classification- isoprene rule- structural determination of citral, Geraniol, Farnesol, α-pinene and camphor.

Alkaloids: Introduction – classification - isolation of alkaloids - total synthesis of quinine, morphine and reserpine.

UNIT-V: CHEMISTRY OF NATURAL PRODUCTS - I I

Nomenclature and classification of heterocyclic compounds - Syntheses of imidazole, oxazole, thiazole, pyrimidines (cytocine and Uaracil only) and purines (adenine, guanine only).

Natural pigments - Synthesis of flavones, isoflavones and anthocyanins,

Steroids - Conversion of cholesterol to progesterone, estrone and testosterone.

Recommended Books

1. J. Dyer, Applicaton of absorption spectroscopy of organic compounds, Prentice Hall of India Pvt. Ltd., New Delhi, 2005.
2. R.M. Silverstein, C.G. Bassler and Monsil, Spectrometric identification of organic compounds, 6th Edn., John Wiley & Sons, New York, 2004.
3. Introduction to the spectroscopic methods for the identification organic compounds - 2 volumes, Schiemann Pergamman Press.
4. I.L. Finar, Organic Chemistry, Volume II, Fifth Edition, First Indian reprint, Pearson Education Asia Pte. Ltd., (2000)
5. S. Kalsi, Spectroscopy of organic compounds, 5th Edn., Wiley Eastern Ltd., Madras, 2002.
6. Jerry March, Advanced Organic Chemistry-Reactions, Mechanisms and Structure, Fourth Edition, John Wiley & Sons (1992)
7. Francis A. Carey, Organic Chemistry, Third Edition, The McGraw-Hill Companies, Inc., 1996.
8. Physical organic chemistry by Neil S. Issac, ELBS publication 1987.
9. Organic reaction mechanism, Macmillan India, 1999.
10. William Kemp, Organic Spectroscopy, ELBS, New Delhi, 1982.
11. Y.R. Sharma, Elementary Organic Spectroscopy, I Edn, S.Chand & Company Ltd, New Delhi, 1980.
12. O.P. Agarwal, Chemistry of Organic Natural Products, Vol I & II, Goel Publishing House, 2014.
13. Terpene Chemistry - James verghese.

PAPER 8

ORGANOMETALLICS & COORDINATION CHEMISTRY

OBJECTIVES:	To study Coordination complexes, Substitution in Coordination complexes and to study Organometallic chemistry and Inorganic photochemistry
COURSE OUTCOME(S)	
CO1	State and show the peculiarities of metal – carbon bond and their structural chemistry.
CO2	Chemical Industry based on the catalytic combination of small molecules like C_2H_4, CO, H_2, H_2O and NH_3 to give larger molecules using organo metallic catalysts revealed.
CO3	Demonstrate reactivity displayed by Co ordination compounds and integrate the usefulness of this reactivity in the synthesis of co ordination compounds
CO4	Describe the importance of Electron transfer Reactions.
CO5	Define the significance of Inorganic photochemistry and apply metal complexes in solar energy conversions.

UNIT-I: ORGANOMETALLIC CHEMISTRY - I

Synthesis, structure and Bonding – Carbon σ donors, synthesis of metal alkyls and Aryls, structure and bonding in metal alkyls and Aryls, metal carbonyls – properties and structure, bonding in carbonyls, carbon π Allyl complexes, structure and bonding in Ferrocene.

Reaction pathways – Association, Substitution addition and elimination reactions – ligand protonation Electrophilic and Nucleophilic attack on Ligands carbonylation and decarbonylation, oxidative addition and fluxional isomerism.

UNIT-II: ORGANOMETALLIC CHEMISTRY - II

Catalysis: Hydrogenation of olefins (Wilkinson's catalyst), hydroformylation of olefins using cobalt or rhodium catalysts (Oxo process), oxidation of olefins to aldehydes and ketones (Wacker process) polymerization (Zeigler - Natta Catalyst); cyclooligomerisation of acetylene using nickel catalyst (Reppe's catalyst);

UNIT-III: COORDINATION CHEMISTRY - IV

Mechanism of Electron Transfer reaction, key ideas concerning electron transfer, outer sphere and inner sphere electron transfer reactions, two electron transfer, formation of precursor complexes, the role of bridging Ligand, Marcus theory- applications.

UNIT-IV: COORDINATION CHEMISTRY - V

Substitution Reactions: Substitution in square planar complexes, reactivity of platinum complexes, influences of entering, leaving and other groups, the trans effect and its theories.

UNIT-V: COORDINATION CHEMISTRY - VI

Substitution Reactions: Substitution of octahedral complexes of cobalt and chromium, replacement of coordinated water, solvolytic (acids and bases) reaction, SN^1, SN^2 & SN^1CB mechanism, applications in synthesis (platinum and cobalt complexes only).

Inorganic Photochemistry: Photo-substitution, Photoredox and isomerisation process, application of metal complexes in solar energy conversion.

TEXT BOOKS

1. R.C. Mehrothra, A. Singh, **Organo Metallic Chemistry**, Wiley Eastern Co., (1992).
2. F. Basolo and R.G. Pearson, **Mechanism of Inorganic Reaction**, Wiley NY (1967).
3. J. Huheey, **Inorganic Chemistry**, Harper and Collins, NY IV Edition, (2009).
4. K.F. Purcell and J.C. Kotz, **Inorganic Chemistry**, W. Saunders Co., (1977).
5. S. FA Kettle, **Coordination Chemistry**, ELBS, (1973).
6. F.A. Cotton and G. Wilkinson, **Advanced Inorganic Chemistry**, John Wiley and Sons, V Edition (1988).
7. D.F. Shrivers, Pw. Atkins and C.H. Langford, **Inorganic Chemistry**, OUP (1990).

8. Guillermo J. Ferraudi, **Elements of inorganic photochemistry**, Wiley (1988).
9. Arthur W. Adamson, Paul D. Fleischauer, **Concepts of inorganic photochemistry**, Wiley(1975).

SUGGESTED REFERENCES

1. G. Coates M.l. Green and K. Wade. **Principles of Organometallic chemistry**, Methven Co., London (1988).
2. P. Powell, **Principles of Organometallic chemistry**, Chappman and Hall. (1998).
3. G.S. Manku, **Theoretical Principles of Inorganic Chemistry**, McGraw-Hill Education, (1984).
4. M.C. Day and J. Selbin, **Theoretical Inorganic Chemistry**, Van Nostrand Co., New York (1974).
5. R.B. Heslop and K. Jones, **Inorganic Chemistry**, Elsevier Scientific Publ., (1976).
6. F. Basolo and R.G. Pearson, **Mechanism of Inorganic Reaction**, Wiley NY (1967).
7. B.E. Dogulas DH McDaniel's and Alexander, **Concepts and Models of Inorganic Chemistry**, Oxford IBH (1983).
8. WU. Mallik, G.D. Tuli, R.D. Madan, **Selected topics in Inorganic Chemistry**, S. Chand and Co., New Delhi (2006).

PAPER - 9

PHYSICAL CHEMISTRY – III

OBJECTIVES:	To study the principle and applications of NMR spectroscopy, the fundamental principles and applications of Quantum chemistry, study of electrode-electrolyte interface and introductory statistical thermodynamics.
COURSE OUTCOME(S)	
CO1	To learn foundations of quantum mechanics and to study the various operators used in Quantum mechanics.
CO2	To study the applications of wave equation to problems like SHO, Rigid Rotator and Hydrogen atom and application of approximation methods.
CO3	To know the basics of Statistical thermodynamics and its applications .To learn about the Maxwell-Boltzmann Statistics and partition function.
CO4	To study the electrode-electrolyte interface, structure of electrical double layers and diffusion.
CO5	To know the fundamentals of NMR spectroscopy and to determine the compound structure using NMR spectra.

UNIT – I: QUANTUM CHEMISTRY – I

Photoelectric effect – Compton Effect – wave-particle duality – uncertainty principle

Theory of wave motion – Wave equation for electrons – Wave function Ψ and its physical significance – condition for acceptable wave function – condition for normalization and orthogonality.

Operator Algebra – Commutative property – linear operator – Eigen values and eigen functions – Hermitian property of operators – Basic postulates of quantum mechanics.

UNIT – II: QUANTUM CHEMISTRY – II

Elementary applications of schrodinger wave equation – Particle in one and three dimensional box – Quantum mechanical results for harmonic oscillator and rigid rotor – Schrodinger equation for hydrogen (No derivation) and the solution – Approximation methods – Variation and Perturbation methods – Application to hydrogen and helium atoms.

UNIT – III: STATISTICAL THERMODYNAMICS – I

Objectives of statistical thermodynamics – Micro states and macro states – Concept of mathematical and thermodynamic probability – Distribution of distinguishable and non-distinguishable particles.

Derivation of Maxwell-Boltzmann distribution law – Partition function – Evaluation of translational, vibrational, rotational and electronic partition function. Expressions for thermodynamic functions in terms of partition function – Applications of partition function to heat-capacity of ideal gases.

UNIT – IV: ELECTROCHEMISTRY - II

Electrode – Electrolyte interface – Adsorption at electrified interface – Electrical double layer – electrocapillary phenomenon – Lippmann equation – Structure of double layers – Helmholtz Perrin; Guoy – Chapmann and stern model of electrical double layers.

Diffusion – Fick's law of diffusion – Effect of ion association on conductance – Electro kinetic phenomena – Membrane potential.

UNIT – V: MAGNETIC RESONANCE SPECTROSCOPY

Resonance spectroscopy – Zeeman effect – Equations of motion of spin in magnetic fields – Chemical shift – Factors affecting chemical shift – Spin – Spin coupling and coupling constant – NMR of simple AX and AMX type molecules – Chemical exchange in NMR – Relaxation process – NMR and Restricted Rotation – C^{13}, ^{19}F, ^{31}P NMR spectra applications – Brief discussion of FT NMR spectroscopy.

TEXT BOOKS

1. S. Glasstone, Introduction to electrochemistry, Affiliated East West Press, New Delhi (1977).
2. P.H. Reiger, Electrochemistry, Chapman and Hall, New York (1994).
3. M.C. Gupta, Statistical thermodynamics, Wiley Easter, New Delhi (1990).

4. S. Glasstone, Text book of physical chemistry (2006).
5. R.K. Prasad, Quantum chemistry, Wiley Eastern, New Delhi (2001).
6. M.W. Hanna, Quantum mechanics, W.A. Benjamin Inc. London (1965).
7. Raymond Chang, Basic principles of spectroscopy, McGraw Hill Ltd., New York (1971).
8. W. Kemp, NMR in chemistry, McMillan Ltd., (3rd Edition, 2008).

SUGGESTED REFERENCES

1. C.N. Banwell, Fundamentals of Molecular spectroscopy, McGraw Hill (4th Edition, 2017).
2. A.K. Chandra, Introductory quantum chemistry, Tata McGraw Hill.
3. D.A. McQuarrie, Quantum chemistry, university science books, Mill valley, California (2nd edition, 2008).
4. J.O.M. Bokris and A.K.N. Reddy, Electrochemistry, Vol. 1 and 2, Plenum, Now York (2nd Edition, 1998).
5. B.J. Meclelland, Statistical thermodynamics, chapman and Hall, London (1973).

ELECTIVE - III

SCIENTIFIC RESEARCH METHODOLOGY

OBJECTIVES:	To study the importance of research, literature survey, error analysis, statistical treatment and to study about the conventions of writing thesis.
COURSE OUTCOME(S)	
CO1	Survey of scientific literature using modern tools explained.
CO2	Separation techniques constitute an important aspect of experimental chemistry and the importance & modern techniques are introduced
CO3	Awareness about the causes of uncertainties in the evaluation of data.
CO4	Scientific data are subjected to mathematical and statistical methods. Elementary treatment of these tests are given
CO5	Set up Skills required to write the thesis report explained.

UNIT-I: SURVEY OF LITERATURE

Nature and importance of Research - Need for Literature Survey – Primary Sources – Secondary Sources – Selection of Research Topic – Selection of Research and Instrumental facilities – Aids of computer devices in literature survey.

UNIT-II: CONDUCT OF RESEARCH WORK

Physical properties useful in analysis and methods of separation prior to analysis - Isolation techniques - extraction - Soxhlet extraction, crystallization, sublimation - methods for vacuum sublimation and distillation under reduced pressure.

Chemistry of working with hazardous materials - acid / water sensitive, corrosive, toxic, explosive and radioactive materials.

UNIT-III: EVALUATION OF ANALYTICAL DATA

Precision and accuracy - Reliability - determinate and random errors - distribution of random errors - normal distribution curve.

UNIT-IV: STATISTICAL ANALYSIS OF DATA

Elimination of outlying Results - Q-Test - T-Test - Statistical Analysis of the T-Test (Null Hypothesis) – The F-Test – Linear Regression – Minimum sum-of-squares – Slope and intercept.

UNIT-V: THESIS WRITING

Components of a thesis – Style and Conventions in writing thesis - The general format –Organization, Title, Summary, Introduction, Experimental procedures, Results and Discussion, Footnotes, Tables, Figures, Chemical and Mathematical usage and References – Write up steps in drafting report.

REFERENCES

1. Douglas A. Skoog and Donald, M. West, Fundamental of analytical chemistry, Halt Saundersons International Edition.
2. J. Anderson,H.M. Durstonand M.Poole, Thesis and assignment writing - Wiley Eastern Ltd., (1970).
3. J. March, Advanced organic chemistry - reactions, Mechanism & Structure. McGraw Hill Student Edition.
4. Vogel’s Textbook of quantitative chemical analysis, ELBS edition.

SEMESTER IV

PAPER - 10

PHOTOCHEMISTRY & BIOORGANIC CHEMISTRY

OBJECTIVES	To understand the concepts of Photochemical Pericyclic Reactions. To learn free radicals reactions, Applications and Techniques of Dyeing, Proteins, Nucleic acids, Antibiotics and Vitamins.
COURSE OUTCOMES	
CO1	To know the principles of photochemistry. To learn their importance pericyclic reactions
CO2	To acquire knowledge about proteins. To know importance of nucleic acids
CO3	To know importance and structural elucidation of antibiotics. To understand the structural characteristics vitamins..
CO4	To know the chemistry of free radicals. To understand the synthetic methods of dyes.
CO5	To know the significance of modern synthetic methods. To understand the chemistry of reactions and reagents.

UNIT-I: PHOTOCHEMISTRY & PERICYCLIC REACTIONS

Photochemical excitation - Fate of the excited molecules - Jablonski diagram - study of photochemical reactions of ketone - photoreduction - photocyclo addition - Paterno - Buchi reaction - di pi-methane rearrangement. Structure of bulvalene, a fluxional molecule - Cope and Claisen rearrangement.

Pericyclic reactions – classification – orbital symmetry – Woodword Hoffman rules - Analysis of electrocyclic, cyclo addition and sigmatropic reactions - correlation diagrams for butadiene – cyclobutene system, hexatriene to cyclohexadiene system, dimerisation of ethylene and Diels-Alder reaction.

UNIT-II PROTEINS AND NUCLEIC ACIDS

Proteins: Peptides and their synthesis – synthesis of tripeptide. Merrifield synthesis, Determination of tertiary, quaternary structure of Protein, Bio-Synthesis of Proteins.

Nucleic Acids: Types of Nucleic Acids-DNA & RNA polynucleotide chain. Components-biological functions. Structure and role of DNA and RNA (Nucleotides only)

Biosynthesis of Cholesterol.

UNIT-III: ANTIBIOTICS & VITAMINS:

Introduction, structural elucidation and synthesis of pencillin, streptomycin and chloromycetin.

Introduction, structural elucidation and synthesis of vitamin A1, vitamin B1 and vitamin B6.

UNIT-IV: FREE RADICALS & DYES

Long and short-lived free radicals, methods of generation of free radicals. Addition of free radicals to olefinic double bonds. The following aromatic radical substitutions are to be studied: decomposition of diazocompounds, phenol - coupling - Sandmeyer reaction Gomberg reaction, Pschorr reaction, Ulmann reaction, mechanism of Hunsdiecker reaction Detection of free radicals by ESR.

Introduction, various methods of dyeing, concept of Chromophore and Auxochrome, classification of dyes, nitroso dyes, Azodyes, - Fast green, Methyl Orange, Methyl Red, Fast Red, tripheylmethane dyes - Malachite green, Rosaniline, Aniline blue, Crystal violet,

Xanthene dyes - Fluorescein, Rhodamine B, Anthraquinone dyes – Alizarin – Preparation and uses.

UNIT – V: MODERN SYNTHETIC METHODS, REACTIONS AND REAGENTS

Synthesis of simple organic molecules using standard reaction like acetylation, alkylation of enamines and active methylene compounds, Grignard reactions, Phosphorus and sulphur ylides Robinson annulation, Diels Alder reactions. Basic principles and terminology of retrosynthesis, 1,2 and 1,3-disconnection approach. Protection and deprotection of functional groups (R-OH, R-CHO, RCO-R, R-NH_2 and R-COOH). Uses of the following reagents: DCC, DDQ, LDA, 1, 3-Dithiane (umpolung) and diisobutylaluminiumhydride (DIBAL).

RECOMMENDED BOOKS

1. Molecular Reaction and Photochemistry by Charles H. Depuy and Orville, L. Champman, Prentice Hall of India Pvt., Ltd., New Delhi.
2. I.L. Finar, Organic Chemistry, Volume II, Fifth Edition, First Indian reprint, Pearson Education Asia Pte. Ltd., (2000)
3. Jerry March, Advanced Organic Chemistry-Reactions, Mechanisms and Structure, Fourth Edition, John Wiley & Sons (1992)
4. Francis A. Carey, Organic Chemistry, Third Edition, The McGraw-Hill Companies, Inc., 1996.
5. Chemistry of organic Natural Products by Dr. O.P. Agarwal, Goel Publishing House, Meerut. (2014).

PAPER – 11

INORGANIC SPECTROSCOPY & ANALYTICAL TECHNIQUES

OBJECTIVES:	To study about the Inorganic Spectroscopy and Analytical techniques.
COURSE OUTCOME(S)	
CO1	UV-Visible, IR, Raman spectral properties of metal complexes, magnetic properties and its measurement methods revealed
CO2	Spectral applications of inorganic systems using NMR, NQR and Massbauer spectroscopy knowledge gained.
CO3	Study about the spectroscopic principles and the properties of ESR and PES
CO4	Learning the spectroscopic analytical techniques of AAS , AES and ICP.
CO5	Gaining knowledge related to analytical techniques of chromatographic and electron microscopic instrumentations.

UNIT-I: INORGANIC SPECTROSCOPY - I AND MAGNETIC PROPERTIES

Applications to inorganic systems of the following: ultra violet, visible, infra-red and Raman spectra of metal complexes, organometallic and simple inorganic compounds.

Magnetic Susceptibility and measurements - Guoy method, Faraday method; applications.

UNIT-II: INORGANIC SPECTROSCOPY – II

Application to Inorganic systems of the followings - NMR, NQR and Mossbauer spectra:

NMR spectra of ^{31}P, ^{19}F, NMR shift reagents.

NQR – structural information.

Mossbauer spectra of Fe and Sn systems.

UNIT-III: INORGANIC SPECTROSCOPY – III

ESR Introduction - Zeeman equation, g-value, nuclear hyperfine splitting, interpretations of the spectrum, simple carbon centered free radicals. Anisotropy - g-value and hyperfine splitting constant. McConnell's equation, Kramer's theorem. ESR of transition metal complexes of copper, manganese and vanadyl complexes.

Photoelectron spectroscopy (UV and X-ray) - photo electron spectra - Koopman's theorem, time structure in PES, chemical shift and correlation with electronic charges.

UNIT-IV: INSTRUMENTAL ANALYSIS – I

Atomic Spectroscopic methods: Introduction – classification of spectral methods

AAS and AES – Principle, instrumentation, spectral and chemical interferences, applications.

Differences between AAS and AES; advantages of AAS over AES.

ICP: Pinciple, instrumentation, interferences and applications.

UNIT-V: INSTRUMENTAL ANALYSIS – II

Chromatography: GLC and HPLC – Principle, instrumentation, working, types of detectors and applications.

Electron Microscopy: SEM, TEM and AFM –Principle, instrumentation and applications.

Text books

1. A. Earnshaw, **Introduction to Magneto Chemistry**, Academic Press, London, (1968).
2. C.N.R. Rao, I.R. Ferraro, **Spectroscopy in Inorganic Chemistry**, Vol. I and Vol. II, Academic Press, (1970).
3. D. A. Skoog and D.M.West, **Principles of Instrumental Methods of analysis**, Saunder's College Publ. III Edition, (1985).

4. E. A. V. Ebsworth, D. W. H. Rankin and S. Cradock, **Structural Methods in Inorganic Chemistry**, II Edition, Blackwell Scientific Publications, Oxford, London (1991).
5. G.D. Christian and J.E.G. Reily, **Instrumental Analysis**, AllegnBecon, II Edition, (1986).
6. H.A. Strobel, **Chemical Instrumentation**, Addison - Wesley Pub. Co., (1976).
7. R. S. Drago, **Physical Methods for Chemists,**Saunders College Publishing, Philadelphia (1992).
8. Willard Merrit, Dean and Settle, **Instrumental methods of analysis**, CBS Publ. VI edition, (1986).

Suggested References

1. AI Vogel, **Text book of Qualitative Analysis** - IV Edition (1985).
2. C. N. Banwell and E.M. Mc Cash, **Fundamentals of Molecular Spectroscopy**. IV edition, Tata McGraw Hill, New Delhi (1994).
3. D.A. Skoog D.M. West, Holt Reinhert and Winston, **Fundamental of Analytical Chemistry**, Publication, IV Edition (1982).
4. D.N. Sathyanarayana, **Electronic Absorption Spectroscopy and Related Techniques,** Universities Press (India) Ltd., Hyderabad (2001).
5. FA Cotton and G Wilkinson, **Advanced Inorganic Chemistry**, John Wiley and Sons, V Edition (1988).
6. G. Aruldhas, **Molecular Structure and spectroscopy**, Prentice Hall of India Pvt. Ltd., New Delhi (2001).
7. J. Huheey, **Inorganic Chemistry**, Harper and Collins, NY, IV Edition, (1993).
8. M.C. Shrivers, P.W Atkins, CH. Langford, **Inorganic Chemistry**, OUP (1999).
9. Nakamoto, **Infrared and Raman Spectra of Inorganic and Coordination Compounds**, IIIEdn., John Wiley and Sons, New York, (1986).
10. O. Khan, **Molecular Magnetism**, New York, VCH (1993).

PAPER – 12

PHYSICAL CHEMISTRY – IV

OBJECTIVES:	To study the applications of quantum chemistry and chemical bonding, types of photophysical processes in chemistry, the mechanism of electrochemical reactions, over potential, corrosion, heat capacity of solids and quantum statistics.
COURSE OUTCOME(S)	
CO1	To know VB and MOT of diatomic and polyatomic molecules, application of HMO to organic molecules.
CO2	To derive Butler-Volmer equation for electron transfer reactions and to know the concept of corrosion and passivation.
CO3	To study the quantum statistics and their application, models of heat capacity of solids.
CO4	To learn about the various photochemical and photophysical processes and to study the kinetics of quenching.
CO5	To understand the various types of photochemical reactions, concept of quantum yield and kinetics of photochemical reactions.

UNIT – I QUANTUM CHEMISTRY – III

Born-oppenheimer approximation – Valence bond theory for hydrogen molecule and hydrogen molecule ion – LCAO – MO theory for diatomic molecules.

Concept of Hybridization - Huckel theory for conjugated molecules (Ethylene, butadiene and benzene) – Semi-empirical methods – Slater orbitals.

UNIT – II ELECTRO CHEMISTRY – III

Mechanism of electrode reaction –Polarisation and over potential – Butler-Volmer equation for one step and multistep electron transfer reactions – Significance of electron exchange current density and symmetry factors – Transfer coefficient and its significance – Mechanism of hydrogen and oxygen evolution reaction.

Corrosion and passivation of metals –Pourbaix diagram – Evan's diagram – Fuel cells.

UNIT – III STATISTICAL THERMODYNAMICS – II

Heat capacity of solids – Einstein and Debye models.

Quantum statistics: Fermi-Dirac and Bose-Einstein statistics and their corresponding distribution functions –Comparison of quantum and classical statistics – Applications of quantum statistics to electron gas in metals and Planck's radiation law.

UNIT – IV PHOTOCHEMISTRY – I

Absorption and emission of radiation – Franck – Condon principle – Decay of electronically excited states –Jablonski diagram – Radiative and non-radiative transitions– Flourescence and phosphorescence

Photophysical kinetics of unimolecular processes – Kinetics of biomolecular process – Static and dynamic quenching – Stern-Volmer equation – Concentration dependence of quenching –Excimer formation.

UNIT – V PHOTOCHEMISTRY – II

Experimental methods – Quantum yield and life time measurements – Steady state principle – Quantum yield and chemical Actinometry.

Kinetics of Photochemical reactions – Hydrogen and halogen reactions,Photolysis of acetaldehyde and dimerization of anthracene.

Photo isomerization, Photo rearrangement, Photo reduction, Photo redox, Photosubstitution and Photosensitized reactions – Aspects of solar energy conversion and storage.

Text Books

1. R.K. Prasad, Quantum chemistry, New age International Publishers, New Delhi (2009).
2. D.A. McQuarrie, Quantum chemistry, university science books, Mill valley, California (1983).
3. N.J. Turro, Modern Molecular Photochemistry, Benjamin, Cumming Mento Park, Univ Science Books; New Ed edition (1991)
4. K.K. Rohatgi, Mukherjee, Fundamentals of Photo chemistry (Revised Edition), Wiley Eastern Ltd. (1992).
5. S. Glasstone, Introduction to electrochemistry, Affiliated East West Press, New Delhi (2006).
6. D.R. Crow, Principles and applications of electrochemistry, Chapman and Hall (1991).
7. M.C. Gupta, Statistical thermodynamics, Wiley Easter, New Delhi (1990).

SUGGESTED REFERENCES

1. J.O.M. Bokris and A.K.N. Reddy, Electrochemistry, Vol. 1 and 2, Plenum, Now York (1977).
2. B.J. Meclelland, Statistical thermodynamics, chapman and Hall, London (1973).
3. A.K. Chandra Introductory quantum chemistry, Tata McGraw Hill.
4. P.W. Atkins, Quantum Mechanics, Oxford university press, Oxford (1983).
5. R.P.Wayne, Photochemistry,Butterworths, London (1970)
6. Francis W Sears and Gerhard L Salinger, Thermodynamics, Kinetic theory and Statistical thermodynamics.

ELECTIVE - IV

ENVIRONMENTAL CEMISTRY

OBJECTIVES:	To study the Atmosphere, Lithosphere, Hydrosphere, and Biosphere - interactions – causes and control of pollution.
COURSE OUTCOME(S)	
CO1	Understand the Environmental issues related to air pollution, classify pollutants, their chemistry and apply abatement methods.
CO2	Recognize the significance of mineral resources and the importance of water as an irreplaceable resource.
CO3	Explain how human activities affect the earth's bio diversity and the impact of ecological disruption on human health.
CO4	State the prospects of Agriculture, describe Agricultural pollution and the significance of carbon and nitrogen cycle.
CO5	Analyze different pollutants and demonstrate the importance of pollution control.

UNIT - I: ATMOSPHERIC CHEMISTRY

The chemistry of air pollution- oxides of nitrogen- hydrogen sulphide and oxides of sulphur- Aerosols – ozone depletion and consequences- dioxins burning plastics- other atmospheric chemicals- smog- radio activity and fallout- air pollution abatement. Green house effect- Global warming, oxides of carbon.

UNIT - II: THE EARTH

The lithosphere- Composition of Lithosphere - Earth resources – Wastes and pollutants in soil and conservation steps.

The hydrosphere: Water pollution– mercury pollution. The chemical constituents of sea water- organic matter and suspended material- ocean dumping- oil pollution. The role of water in our total environment.

UNIT - III: THE BIOSPHERE

The structure of the biosphere, Man's perturbation of the biosphere – Man as a chemical factory – material use and waste – energy use and thermal pollution – ecological disruption – chemical sensation, hormonal imbalance and mutagens.

UNIT IV: INTERACTIONS

Lithosphere- biosphere interaction: soil chemistry – the prospects of agriculture- agricultural pollution – pesticides and other persistent pollutants – the deposition of coal and petroleum –the nitrogen cycle – the carbon cycle – air – sea interactions.

UNIT - V: POLLUTION CONTROL

Pollution control in the following: Fertilizer, petroleum, pulp and paper, tanning, sugar, alcohol, electroplating and nuclear reactors.

Analysis of pollutants: Sum, specific and group parameters BOD, COD, Fe, Cr, Cu, Pb, and Ni-$SO_2$and NOx.

A total of 20% syllabus change has been made in units I, II, III, and IV.

REFERENCES

1. R.A. Horne, Chemistry of our environment, Wiley Interscience Publications, New York (1978).
2. A.K. De, Environmental chemistry, New Age International Private Ltd. (2017)
3. Jain L, Marr and Malcom S. Cresser Environmental chemical analysis, Bishopbriggs, Glassgow International Textbook Co., NewYork (1983).

4. S.P. Mahajan, Pollution control in process industries, Tata Mcgraw – Hill Education (1985).

MAIN PRACTICAL

PRACTICAL IV

ORGANIC CHEMISTRY PRACTICAL – II

OBJECTIVES	To understand the principles of various types of titrimetric analysis. To know the significant figures and various errors. To become aware of handling of glass wares used in laboratory. To acquire the skills of doing quantitative estimations by titrimetry. To know the spectral methods of identifying the structure of organic compounds.

I. Any six preparations from the following involving two stages

1. sym-Tribromo benzene from aniline.
2. Benzanilide from benzophenone
3. m-Nitro benzoic acid from methyl benzoate
4. 2,4- Dinitrobenzoic acid from p-nitrotoluene
5. m-Nitro benzoic acid from benzaldehyde
6. Benzil form benzaldehyde
7. Anthraquinone from phthalic anhydride
8. Anthranilic acid from phthalic acid
9. 2-Phenyl indole from phenyl hydrazine
10. 2, 4-dinitrophenyl hydrazine from p-nitrochlorobenzene

II. Any two exercises in the extraction of natural products (Not for examination)

1. Caffeine from tea leaves
2. Lactose from milk

3. Citric acid from lemon
4. Piperine from black pepper

III. Chromatographic separations (Not for examination)

1. Column chromatography: Separation of anthracene and picric acid from anthracene picrate.
2. Thin layer chromatography: Separation of green leaf pigments.
3. Paper chromatography: Identification of amino acids.

IV. Any five estimations

1. Estimation of aniline
2. Estimation of phenol
3. Estimation of ethyl methyl ketone
4. Estimation of glucose
5. Estimation of amino group
6. Estimation of amide group
7. Saponification of fat or an oil
8. Iodine value of an oil

V. Special interpretation of organic compounds UV, IR, PMR and mass spectra of the following 15 compounds

1. 1,3,5- Trimethyl benzene
2. Pinacolane
3. n-Propylamine
4. p-Methoxy benzyl alcohol
5. Benzyl bromide
6. Phenyl acetone
7. 2-Methoxyethyl acetate
8. Acetone
9. Isoopropyl alcohol
10. Acetaldehyde diacetate
11. N,N-Dimethylamino ethanol
12. Pyridine
13. 4-Picoline
14. 1,3-dibromo - 1, 1- dichloropropene
15. Cinnamaldehyde

Recommended Books

1. Arthur I.Vogel, A text book of Practical Organic Chemistry, ELBS
2. Raj K. Bansal, Laboratory Manual of Organic Chemistry, Wiley Eastern limited.
3. N.N. Greenwood and A. Earnshaw, Chemistry of the Elements, Vol.II, Pergamon Press (1997).

TOTAL MARKS FOR PRACTICAL PAPER = 100 MARKS

University Examination	Marks	Internal Assessment	Marks
Estimation	30	Two Tests	10
Preparation	20	Attendance / Regularity	10
Interpretation of spectra	10	Results accuracy	05
Record	05	**Total**	**25**
Viva voce	10		
Total	**75**		

PRACTICAL V

INORGANIC CHEMISTRY PRACTICALS – II
QUANTITATIVE ANALYSIS OF COMPLEX MATERIALS

a) ANALYSIS OF ORES

1. Determination of percentage of calcium and Magnesium in dolomite.
2. Determination of percentage of MnO_2 in pyrolusite.
3. Determination of percentage of lead in galena.

b) ANALYSIS OF ALLOYS

1. Estimation of tin and lead in solder.
2. Estimation of copper and zinc in brass.
3. Estimation of chromium and nickel in stainless steel.

c) ANALYSIS OF INORGANIC COMPLEX COMPOUNDS

1. Preparation of cis and trans potassium bis (oxalato) diaquochromate(III) and analysis of each of these for chromium.
2. Preparation of potassium tris (oxalato) ferrate (III) and analysis for iron and oxalate.

d) QUANTITATIVE ANALYSIS

Quantitative analysis of mixtures of iron-magnesium; iron - nickel; copper - nickel and copper - zinc.

e) COLORIMETRIC ANALYSIS

(Using) Photoelectric method: Estimation of iron, nickel, manganese and copper.

f) BIAMPEROMETRIC TITRATIONS

(With dead stop endpoint) thiosulpate - iodine system and Iron (II) - cerium (IV) systems.

g) LIST OF SPECTRA TO BE GIVEN FOR INTERPRETATION.

1. ^{31}p NMR Spectra of methylphosphate
2. ^{31}p NMR Spectra of HPF_2
3. ^{19}F NMR Spectra of CIF_3
4. ^{1}H NMR Spectra of Tris (ethylthioacetanato) cobalt (III)
5. Explain high resolution ^{1}H NMR spectra of (N-propylisonitrosoacetylacetoneuninato) (acetylacetonato) Nickel (II)
6. ESR Spectra of the aqueous $ON(SO_3)^{2-}$ ion.
7. ESR Spectra of the H atoms in CaF_2.
8. ESR Spectra of the $[Mn (H_2O)_6]^{2+}$.
9. ESR Spectra of the bis (salicylaldiminato) copper (II)
10. IR Spectra of the sulphato ligand.
11. IR Spectra of the dimethylglyoxime ligand and its Nickel (II) complex.
12. IR Spectra of carbonyls
13. Mossbauer spectra of $FeSO_4$ $7H_2O$
14. Mossbauer spectra of $FeCl^{3.}$
15. Mossbauer spectra of$[Fe(CN)_6]^{3-}$
16. Mossbauer spectra of $[Fe (CN)_6]^{4-}$

TOTAL MARKS FOR PRACTICAL PAPER = 100 MARKS

SEMESTER EXAMINATION	**Marks**
I. Estimation of mixture containing two metal ions	
Volumetric	15
Gravimetric	10
Procedure	5(3+2)
II. Colorimetric estimation / amperometric titration	
Estimation	15
Procedure	05
III. Interpretation of Spectra	10
Record	05
viva-voce	10
Total	**75**

INTERNAL ASSESSMENT	**Marks**
Two Tests	10
Attendance / Regularity	10
Results accuracy	05

Total	**25**

PAPER-6

PHYSICAL CHEMISTRY PRACTICAL- II

Experiments in electrochemistry: conductometry, potentiometry, pH metry and spectroscopy.

CONDUCTIVITY MEASUREMENTS

Determination of equivalent conductance of a strong electrolyte and verification of Debye - Huckel - Onsager Equation
Verification of Debye-Huckel limiting law
Verification of Ostwald's Dilution law for a weak electrolyte. Determination of PK values of weak acids and weak bases.
Conductometric titrations between acid (simple and mixture of strong and weak acids) - base, precipitation titrations including mixture of halides.

E.M.F MEASUREMENTS

Determination of standard potentials (Copper & Zinc)
Determination of thermodynamic quantities from EMF measurements - potentiometric titrations.
Determination of pH and calculation of pKa.
Determination of stability constant of a complex.
Determination of solubility product of a sparingly soluble salt. Redox titrations.
Precipitation titration of mixture of halides by EMF measurements.

SPECTROSCOPY

Experiments given only to familiarize the interpretation of spectra provided. Interpretation of simple UV-Visible spectra of simple molecules for the calculation of molecular data and identification of functional groups (5 typical spectra will be provided).
IR and NMR spectral calculations of force constant - identification and interpretation of a spectra (5 each in IR and NMR will be provided).

LIST OF EXPERIMENTS SUGGESTED FOR PHYSICAL CHEMISTRY PRACTICAL II

Typical list of possible experiments are given. Experiments of similar nature and other experiments may also be given. The list given is only a guideline. Any 15 experiments have to be performed in a year.

1. Determination of the equivalent conductance of a weak acid at different concentrations and verify Ostwald's dilution law and calculate the dissociation constant of the acid.
2. Determination of equivalent conductance of a strong electrolyte at different concentrations and examine the validity of the Onsager's theory as limiting law at high dilutions.
3. Determination of the activity co-efficient of Zinc ions in the solution of 0.002M Zinc sulphate using Debye-Huckel limiting law.
4. Determination of the solubility product of silver bromate and calculate its solubility in water and in 0.01 M KBrO3 using Debye-Huckel limiting law.
5. Conductometric titrations of a mixture of HCl, CH_3COOH and $CuSO_4$ and NaOH.
6. Determination of the dissociation constant of an acid at different dilution.
7. Determination of the solubility of the lead iodide in water , 0.04 M KI and 0.04 M Pb(NO3)2 at 298 K
8. Determination of the solubility product of leadiodide at 298 K and 308 K and calculate the molar heat of solution of lead iodide.
9. Compare the relative strength of acetic acid and mono chloroacetic acid by conductance method.
10. Determine the basicity of organic acids (oxalic /benzoic).
11. Study the effect of solvent on the conductivity of $AgNO_3$/acetic acid and determine the degree of dissociation and equilibrium constant in different degree of dissociation and mixtures (DMSO, DMF, dioxane, acetone, water) and test the validity of Debye-Huckel Onsager's equation.
12. Determine the solubility of $Ca(TiO_3)_2$ in deionised water and in dilute solution of KCl at 298 K. Determine the solubility product graphically.
13. Determine the equivalent conductivity of a Ca electrolyte and dissociation constant of the electrolyte.
14. Determine the equivalent dissociation constant of a polybasic acid.
15. Determine the electrode potentials of Zn and Ag electrodes in 0.1M and 0.001M solutions at 298 K and fine the standard potentials for these electrodes and test the validity of Nernst equation.
16. Determine the activity co-efficient of an electrolyte at different molalities by EMF measurements.
17. Determine the dissociation constant of acetic acid titrating it with sodium hydroxide using quinhydrone as an indicator electrode and calomel as a reference electrode.
18. Study of the electrolytic separation of metals (Ag, Cu, Cd and Zn)
19. Determine the strength of a given solution of KCl using differential potentiometric titration technique.
20. Determine the dissociation constant of acetic acid in DMSO, DMF, acetone and dioxane by titrating it with KOH.
21. Determine the transport number of cadmium ions and sulphate ions by measuring emf of concentration cells with and without transference.
22. Determine the dissociation constant of monobasic or dibasic acid by all the Alber-Serjeant method.
23. Determine the transport number of Ag ions and nitrate ions by Hittorf's method.

24. Calculate the $ZnSO_4 + H_2$ by emf method and thermodynamic parameters for the reaction $Zn + H_2SO_4$
25. Determine the formation constant of silver-ammonia complex and stoichiometry of the complex potentiometrically.
26. Determine the pH of the given solution with the help of indicators using buffer solutions and by colorimetric method.
27. Perform acid-base titration in a non aqueous medium.
28. Determine pH value of an acid-base indicator (methyl red) by colorimetry.
29. Determine the composition and instability constant of a complex by mole ratio method.
30. By colorimetry determine simultaneously Mn and Cr.
31. Determine lead ion by amperometric titrations with potassium dichromate.
32. Determine ferric ion by amperometric titration.
33. Determine the stability constant of a complex by polarographic method.
34. Estimate the concentration of cadmium and lead ions by successive reduction in polarography. Verify Illkovic equation.
35. Determine the g value from a given ESR spectrum.

Quantum of marks in respect of Practical Examinations

University Examination	**Marks**	**Internal Assessment**	**Marks**
Procedure	10	Two Tests	10
Manipulation	25	Attendance / Regularity	10
Result	15	Results accuracy	05
Interpretation of spectra	10	**Total**	**25**
Record	05		
Viva voce	10		
Total	**75**		