MANONMANIAM SUNDARANAR UNIVERSITY
TIRUNELVELI
PG - COURSES – AFFILIATED COLLEGES
Course Structure for M.Sc. Chemistry
(Choice Based Credit System)
(with effect from the academic year 2017- 2018 onwards)

Sem. (1)	Sub. No. (2)	Subject Status (3)	Subject Status (3)	Hrs/ week Contact (5)	Credits (6)
III	15	Core - 13	Organic Chemistry – III	5	4
	16	Core - 14	Inorganic Chemistry – III	5	4
	17	Core - 15	Physical Chemistry – III	4	4
	18	Core - 16	Scientific - Research Methodology	4	4
	19	Core - 17 Practical - 7	Organic Chemistry Practical – III	4	2
	20	Core - 18 Practical - 8	Inorganic Chemistry Practical – III	4	2
	21	Core - 19 Practical - 9	Physical Chemistry Practical – III	4	2
IV	22	Core - 20	Organic Chemistry – IV	4	4
	23	Core - 21	Inorganic Chemistry – IV	4	4
	24	Core - 22	Physical Chemistry – IV	4	4
	25	Core - 23 Practical - 10	Organic Chemistry Practical – IV	4	2
	26	Core - 24 Practical - 11	Inorganic Chemistry Practical – IV	4	2
	27	Core - 25 Practical - 12	Physical Chemistry Practical – IV	4	2
	28	Core - 26	Project	6+6*	6

SECOND YEAR

(2017- 2018 onwards)

THIRD SEMESTER THEORY

Components	Sub.Code	Contact Hrs / Week	Credits	Internal Marks	External Marks	Total Marks	Passing Minimum	
							External	Total
Core – 13 Organic Chemistry - III	PCHM31	5	4	25	75	100	38	50
Core – 14 Inorganic Chemistry -III	PCHM32	5	4	25	75	100	38	50
Core – 15 Physical Chemistry- III	PCHM33	4	4	25	75	100	38	50
Core – 16 Scientific- Research Methodology	PCHM34	4	4	25	75	100	38	50

THIRD SEMESTER PRACTICAL

Components	Sub.Code	Contact Hrs / Week	Credits	Internal Marks	External Marks	Total Marks	Passing Minimum	
							External	Total
Core – 17 Organic Chemistry practical –III	PCHL31	4	2	50	50	100	25	50
Core – 18 Inorganic Chemistry practical-III	PCHL32	4	2	50	50	100	25	50
Core – 19 Physical Chemistry practical- III	PCHL33	4	2	50	50	100	25	50

FOURTH SEMESTER THEORY

Components	Sub.Code	Cont. Hrs / Week	Credits	Internal Marks	External Marks	Total Marks	Passing Minimum	
							External	Total
Core – 20 Organic Chemistry -IV	PCHM41	4	4	25	75	100	38	50
Core – 21 Inorganic Chemistry-IV	PCHM42	4	4	25	75	100	38	50
Core – 22 Physical Chemistry-IV	PCHM43	4	4	25	75	100	38	50

FOURTH SEMESTER PRACTICAL

Components	Sub.Code	Contact Hrs / Week	Credits	Internal Marks	External Marks	Total Marks	Passing Minimum	
							External	Total
Core – 23 Organic Chemistry practical –IV	PCHL41	4	2	50	50	100	25	50
Core – 24 Inorganic Chemistry practical-IV	PCHL42	4	2	50	50	100	25	50
Core – 25 Physical Chemistry practical- IV	PCHL43	4	2	50	50	100	25	50
Core-26 Project & viva- voce	PCHP41	6+6*	6	50	50	100	25	50

*Extra hours for the project

For the project, flexible credits are b/w 5-8 & Hours per week are b/w 10-16.

Total number of credits ≥ 90 : 90

Total number of Core Courses : 26 (13T+12P+1Project)

Total number of Elective Courses : 02

Total number of Courses : 28

Total hours : 120

Evaluation

The evaluation for each course consists of two components that are internal and external.

Theory

External : Internal = 75:25

Practical

External : Internal = 50:50

INTERNAL

The internal component consists of following:

THEORY

Regarding the internal assessment, the maximum 25 marks is allocated in the following manner.

Components	Marks
The average of the best two tests From three compulsory tests	15
Assignment	4
Seminar	6
Total	25

Note : Re internal assessment test for the student will not be allowed

PRACTICAL

The break-up for the internal component for the practicals will be as follows.

Number of experiments	=	30
Record	=	10
Mid-term test and Model test average	=	10
Total		50

EXTERNAL

Theory

The external evaluation will be based on the examinations to be conducted by the university at the end of each semester.

Question Pattern

Section – A (10 x 1= 10 Marks)
Answer **ALL** the Questions(Multiple choice questions)

Section – B (5 x 5 = 25 Marks)
Answer **ALL** the questions Choosing either (a) or (b)

Section – C (5 x 8 = 40 Marks)
Answer **ALL** questions choosing either (a) or (b)

Total = 75

Practical

Practical examinations will be conducted at the end of the each semester. The scheme of valuation is to be decided by the respective board of questions setters.

Project and Viva – Voce

Project report evaluation and Viva-Voce will be conducted by the external examiner and the guide. The break up for the project work is:

Components	Marks
Project Report	30
Viva – Voce	20
Total =	50

Note :

Scheme of valuation of thesis included, choosing a universal problem, novelty of the title, purpose and importance of research for future development and sustainable, methodology of writing thesis and journal articles etc.

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ORGANIC CHEMISTRY – III

Objectives:

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1. To understand the Aliphatic Nucleophilic substitutions, concept of NMR, Mass Spectroscopy.
2. To understand the photochemistry, pericyclic and Hetero cyclic reactions.

Unit-I : Aliphatic nucleophilic substitution and Elimination Reactions: (15 Hours)

Aliphatic nucleophilic substitution : Mechanism of S_N1, S_N2, S_Ni, S_N1', S_N2' and S_Ni' reactions- Effect of substrate, nucleophile, leaving group and solvent on the rate of substitution- Ambident nucleophile- NGP- Mechanism of esterifications and ester hydrolysis ($B_{AC}2$ and $A_{AC}2$ mechanisms only)

Elimination reaction: E_1, E_2 and E_1CB mechanisms- Factors influencing elimination reactions- Hofmann and Satyzeff rules- Pyrolytic elimination- Chugaev and cope reactions- competition between substitution and elimination reactions.

Unit – II: NMR SPECTROSCOPY (15 Hours)

^{1}H-NMR spectroscopy: Basic Principle – number of signals – chemical shift – Factors influencing chemical shift - spin–spin splitting–Proton exchange reactions - classification of spin systems – analysis of AX, AMX and ABX systems – Geminal, Vicinal and long range couplings–NOE in stereochemistry – FTNMR.

C-13 spectroscopy: Principle of proton decoupled and OFF- resonance decoupled C-13 spectroscopy - comparison with H^1NMR - chemical shifts (aliphatic, olefinic, alkynic, aromatic and carbonyl compounds)

2D NMR spectroscopy: H^1–H^1COSY, H^1–C^{13} COSY, NOESY, DEPT and INADEQUATE spectra.

Unit – III: MASS SPECTROSCOPY (15 Hours)

Basic Principles– Base peak – molecular ion – nitrogen rule – metastable ions – isotopic peak - daughter ions – Mc–Lafferty rearrangement – RDA – General rules for fragmentation pattern – Fragmentation pattern of simple compounds of hydrocarbons, alcohols, amines, aldehyde, ketone, ether, acids, phenols ,nitro compounds, alicyclic compounds .

Alternative electron impact ionization technique– CI, FAB, ESI – MS, MALDI –MS, MALDI-TOF , ICP- MS.

One conjunction problem based on UV, IR, H^1 NMR, ^{13}C NMR and Mass spectroscopic techniques is compulsory under section – c. Problems shall be based on the reference books.

Unit-IV : Organic photochemistry and pericyclic reactions (15 Hours)

Organic photochemistry: Jablonskii diagrams-intersystem crossing-energy transfer process-Photosensitization- alpha cleavages or Norrish type-I and Norrish Type II cleavages - Paterno-Buchi reactions- Barton reaction, cis-trans isomerisation. - Di-π methane rearrangement.

pericyclic reactions:

Atomic and molecular orbitals-Woodward-Hoffmann rules, FMO and correlation diagram approaches:

Electrocyclic reaction: con and dis rotatory motions for 4n and 4n+2system (butadiene and 1,3,5-hexatrienes)- Stereochemical course of electro cyclic reaction in terms of conservation of orbital symmetry.

Cycloaddiation: suprafacial and antarafacial, [2+2] and [4+2] cyclo addition reactions (ethylene and butadiene)

Sigmatropic rearrangements - [i,j] shift of C-H and C-C bonds (1,3) and (1,5) carbon migration.

Unit-V : Heterocyclic and biomolecules (15 Hours)

Synthesis and reactions of indole, oxazole, imidazole, thiazole, Reserpine and quinine chromans, pyrimidine, pyridazine, pyrazine, coumarins, benzopyrones and anthocyanins-synthesis of flavones, isoflavones, flavonol, and quercetin -Biosynthesis of flavonoids. Synthesis

Pyranose and furanose forms of aldohexose and ketohexose-methods used for the determination of ring size-A Detailed study on the structure of maltose, lactose and starch.

REFERENCES

1.J.March, ‘ Advanced organic chemistry’, Fourth Edition, John Wiley and Sons, Newyork, 2006.
2. Depuy, E.C.H. and Chapman, O.S., “Molecular reactions and photochemistry” , Prentice Hall, New York, 1988.

3.I.L. Finar, 'Organic Chemistry', volume 2, sixth Edition, Pearson Education Inc., Singapore, 2006.

4.Raj K. Bansal, 'Organic Reaction mechanisms", Tata Mc Graw Hill, Third Editon, 2007

5.Singh, J., and Singh, J., "Photochemistry and Pericyclic reaction", New Age International, New Delhi, 2004

6.H.O. House, 'Modern synthetic Reaction,'Second Edition , W.A. Benjamin, Inc., London, 1972

7.R.K. Mackie, M.M. Smith and R.A. Aitken,'Guide Book to Organic Synthesis' Second Edition, Longman Seientific and Technical, Singapore, 1990.

8.Carrutherus , W., " Some Modern Methods in Organic Syntheis", Third edition, Cambridge University Press, New York, 1997.

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11.P. Sykes, 'A Guide book to mechanism in organic chemistry', Orient Longman, 1989.

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Himalaya publishing House, Bombay 1992.

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14.R.O.C .Norman, Principles of organic synthesis- Chapman and hall, London.

15.De Mayo, Molecular rearrangements

16. E.S. Gould, 'Mechanism and structure in organic chemistry' Holt, Rinehart and

Winston Inc., 1959

17. F.A. Carey, Organic chemistry – Tata Mc Graw Hill, Delhi, 5th edition 2005.

18. Stryer, L., "Biochemistry", Fifth edition, W.H.Freeman and company, San Francisco, 2002.

19. Jain, J.L., "Fundamentals of Biochemistry",Fourth edition, S.Chand & Company Limited, New Delhi.2007

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INORGANIC CHEMISTRY - III

Objectives:

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- *To introduce organometallic compounds and to study their catalytic applications in homogeneous and heterogeneous systems.*
- *To study the applications of NMR and EPR techniques in inorganic systems.*
- *To understand the basic principles and applications of thermo and spectro analytical techniques.*
- *To introduce inorganic photochemistry and to study applications in various systems.*

Unit I – ORGANOMETALLIC CHEMISTRY – I (15 Hours)

The 18 e^- and 16 e^- rules and its correlation to stability – Synthesis and structures of metal carbonyls, metal nitrosyls and dinitrogen complexes – Substitution reactions of metal carbonyls - IR spectralapplications – identifications of bridging and terminal CO groups – Stretching mode analysis of metal carbonyls – evidence for M-M bonds. Synthesis, properties and structural features of metal complexes with alkene, alkyne, allyl andarene systems. Metallocenes – synthesis, properties, structure and bonding with particular reference to ferrocene and berryllocene – covalent versus ionic bonding in beryllocene. Template synthesis of macrocyclic ligands.

Unit II – ORGANOMETALLIC CHEMISTRY – II (15 Hours)

Organometallic compounds as catalysts and the requirements: Agostic interaction – Oxidative addition and reductive elimination - insertion and elimination reactions – nucleophilic and electrophilic attack of coordinating ligands - cyclometallation reactions. **Homogeneous catalysis:** Wilkinson's catalyst and hydrogenation reactions, Tolman catalytic loop; hydroformylation (oxo) reaction, Wacker and Monsanto acetic acid processes. Cluster compounds, polymer-supported and phase-transfer catalysis. **Heterogeneous catalysis:** synthesis gas and water gas shift reactions; Fischer Tropsch process and synthetic gasoline, Ziegler-Natta polymerization and mechanism of stereoregular polymer synthesis. Cyclooligomerisation of acetylenes (Reppe's or Wilke's catalyst) – Olefin isomerisation using Ni catalyst – olefin metathesis catalysed by Schröck type carbene.

UNIT-III: SPECTRAL METHODS TO THE STUDY OF INORGANIC COMPOUNDS – I (15 Hours)

NMR SPECTROSCOPY: ^{31}P, ^{19}F and ^{15}N – NMR – applications in structural problems based on number of signals, multiplicity, anisotropy (like H_3PO_3, H_3PO_2, $[HNi(PPh_3)_4]^+$, SF_4, TiF_4, PF_5, HPF_2, H_2PF_3, $PF_3(NH_2)_2$, P_4S_3, $P_4N_4Cl_6(NHC_6H_5)_2$, $P_3N_3(CH_3)_2Cl_4$, NF_3, NH_3 – mer- and fac-$Rh(PPh_3)_3Cl_3$, fluxional molecules (including organometallic compounds) and study of fluxionality by NMR technique - NMR of paramagnetic molecules - contact shifts. Evaluation of rate constants - monitoring the course of reaction using NMR.

EPR spectroscopy: Factors affecting magnitude of g-values - Zero field splitting and Kramers' degeneracy - Application of EPR in the study of transition metal complexes based on number of signals, multiplicity, anisotropy (bis(salicylaldimine)copper(II), $[Cu(bpy)_3]^{2+}$, $[Cu(Phen)Cl_2]$, $[(NH_3)_5Co\text{-}O_2\text{-}Co(NH_3)_5]^{5+}$, $Co_3(CO)_9Se$, $Co_3(CO)_9Rh$, $[CoF_6]^{4-}$, $[CrF_6]^{3-}$, $VO(acac)_2$, $[VO(H_2O)_6]^{2+}$, $[Fe(CN)_5NO]^{2-}$). Applications in predicting the covalent character of M-L bond and Jahn-Teller distortion in Cu(II) complexes. EPR spectroscopy of metallobiomolecules: copper and iron proteins.

UNIT – IV: THERMOANALYTICAL AND SPECTROANALYTICAL METHODS (15 Hours)

Theory and principles of thermogravimetric analysis, differential thermal analysis and differential scanning colorimetry – characteristic features of TGA and DTA curves – factors affecting TGA and DTA curves – complementary nature of TGA and DTA – applications of thermal methods in analytical chemistry – thermometric titrations – the study of minerals and metal compounds. Principle and applications of spectrophotometry, spectrofluorimetry, atomic absorption spectroscopy and atomic emission spectroscopy based on plasma sources.

UNIT -V : PHOTOCHEMISTRY OF METAL COMPLEXES (15 Hours)

Frank Condon and thermally equilibrated excited (THEXI) states – properties of excited states of metal complexes – types of excited states, photophysical processes: bimolecular deactivation and energy transfer, photochemical processes: electron transfer reactions, isomerisation and substitutional processes – Photochemistry of Cr(III) and Co(III) complexes – Photophysical and photochemical properties of $[Ru(bpy)_3]^{2+}$. Applications of inorganic photochemistry: photochemical conversion and storage of solar energy – inorganic

photochemistry at semi-conductor electrodes - Catalyzed photoreduction of CO_2 and CO – TiO_2 as a green photocatalyst in removing air and water pollutants.

REFERENCES

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10. Russell S. Drago, *Physical Methods for Chemists*, Surfside Scientific Publishers, 2nd Edition, 1977.
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12. David W. H. Rankin, Norbert W. Mitzel, Carole A. Morrison, *Structural Methods in Molecular Inorganic Chemistr*y, John Wiley & Sons, Ltd, 1st Edition, 2013.
13. Robert A. Scott and Charles M. Lukehart, *Applications of Physical Methods to Inorganic and Bioinorganic chemistr*y, John Wiley & Sons Ltd, 2007.

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15. John A. Weil, James R. Bolton, *Electron Paramagnetic Resonance Elementary Theory and Practical Applications*, 2nd Edition, John Wiley & Sons, 2007.
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PHYSICAL CHEMISTRY- III

Objective: L T P C
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Learning the concepts of Group Theory

To understand the Principles and applications of various spectroscopy

UNIT-I: Group Theory-I (12 Hours)

Symmetry elements and operations. Group Postulates and types of groups. Identification of Point groups of molecules and Schoenflies symbols. Construction of multiplication table for C_{2v}, C_{3v} and C_{2h}. Sub-groups and classes of symmetry operations. Rule of similarity transformations. Matrix representations of symmetry operations. Use of atomic wave functions as bases for point group representations. Reducible and irreducible representations. The Great Orthogonality theorem. Properties of Reducible and irreducible representations. Construction of character tables for C_{2V}, C_{3V}, C_{4V}, C_{2h}, and D_2 point groups by using The Great Orthogonality theorem.

UNIT-II : Group Theory -II : (12 Hours)

Standard Reduction Formula, Vibrational modes as bases for group representations-Normal mode analysis for non linear molecules H_2O, $POCl_3$, trans-N_2F_2 and $PtCl_4$. Symmetry selection rules for infrared and Raman spectra. Mutual exclusion principle. Determination of Hybridisation of atomic orbitals in non-linear molecules (CH_4, XeF_4, and PF_5). Electronic spectra of ethylene and formaldehyde molecules. Construction of Projection operators and Molecular orbitals by Symmetry Adapted Linear Combinations. Simplification of HMO calculations using group theory. Calculation of delocalization energy for ethylene, trans-1,3 – butadiene, and benzene systems.

UNIT – III: Nuclear Magnetic Resonance Spectroscopy (12 Hours)

Theory of Proton NMR spectroscopy, Chemical shift and its measurement, Factors influencing chemical shift, Solvents used in NMR, solvents shift-concentration and temperature effects-hydrogen bonding. Theory of Spin-spin splitting-Magnitude of coupling-coupling constants, J, First-order spectra of complex systems, chemical and magnetic equivalence in NMR, Proton exchange reactions, Factors influencing coupling constant, J. Theory and Principle of ^{13}C, ^{19}F, ^{31}P NMR-Range of chemical shift values, spectra of typical

examples. FT NMR-FIDs. Theory of Spin-spin splitting and double irradiation, InterNuclear Double Resonance (INDOR) and Selective Population Inversion (SPI), Nuclear Overhauser Effect (NOE), 2D NMR-shift correlation spectra-COSY, Magnetic Resonance Imaging (MRI).

UNIT-IV: NQR and EPR spectroscopy (12 Hours)

Electron paramagnetic resonance spectroscopy: theory of EPR spectroscopy, presentation of the spectrum, nuclear hyperfine splitting in isotropic systems. EPR spectra of anisotropic systems: anisotropy in g-value, causes of an isotropy, anisotropy in hyperfine coupling. Double resonance in ESR, Zero field splitting and Kramers' degeneracy.

Theory and Principle of NQR spectroscopy-Nature of electric field gradient, Energy levels and selection rules, Interaction of electric quadrupole with electromagnetic radiation, nuclear orientations, the asymmetry parameter, quadrupole transitions in spherical, axially symmetric fields and not axially symmetric fields. Applications of NQR spectra.

UNIT-V: Electronic Spectroscopy, Mossbauer Spectroscopy and Mass Spectrometry (12 Hours)

Electronic Spectroscopy-Electronic Spectrum of diatomic molecules-Born-Oppenheimer approximation, Progressions, Franck-Condon Principle, Dissociation Energy and dissociation products, Rotational Fine structure of Electronic-Vibration Transitions, The Fortrat diagram, Predissociation, Electronic states of atoms, Electron orbitals in diatomic molecules, Electronic states of diatomic molecules, Potential energy curves for Electronic states of diatomic molecules.

Photoelectron Spectroscopy-Basic Principles, Ultra-Violet Photoelectron Spectroscopy, X-ray Photoelectron Spectroscopy, Chemical information from Photoelectron Spectroscopy.

Mössbauer spectra: Theory and Principle of Mössbauer spectra, isomer shift, quadrupole interactions, magnetic hyperfine interaction, Doppler shift, recoil energy, experimental technique-sources, absorber, calibration, Chemical applications.

Mass spectrometry: Operation and representation of spectra. Effect of combination of high energy electron with a molecule. Finger print application and the interaction of mass spectra, Effect of isotopes on the appearance of a mass spectrum, Molecular weight determinations.

REFERENCE BOOKS

1. Introductory Group Theory For Chemists- George Davidson

2. F. Albert Cotton, Chemical Applications of Group Theory, Third Edition John Wiley & Sons, Singapore 2003.
3. V. Ramakrishnan and M. S. Gopinathan: Group Theory in chemistry, Vishal Publication, 1986.
4. Robert L. Carter, Molecular Symmetry and Group Theory John Wiley and Sons, Inc., New York, 1998.
5. R.L. Flurry, Jr, Symmetry Groups – Prentice Hall, New Jersy 1980.
6. Group Theory and its applications to Chemistry by K. V. Raman
7. Group Theory and Spectroscopy by K. Veera Reddy
8. Group Theory and its Chemical applications by B.K. Battacharya
9. C.N. Banwell and E. M. McCash, Fundamentals of Molecular Spectroscopy, 4th ed., Tata McGraw Hill, New Delhi, 2000.
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12. Organic spectroscopy, William Kemp, Third Edition.
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SCIENTIFIC - RESEARCH METHODOLOGY

L T P C

Objectives: 4 0 0 4

- *How to learn the survey for literature, chemical abstract, choosing a research problem and scientific writing, characterization and data analysis, computer searches and literature.*
- *How to apply for the various finding agencies.*

Unit – I: LITERATURE SURVEY (12 Hours)

Source of chemical information – primary, secondary, tertiary sources-literature survey-Indexes and abstracts in science and technology – Applied science and technology index, chemical abstracts, chemical titles, current chemical reactions, current contents and science citation index.

Classical and comprehensive reference works in chemistry-synthetic methods and techniques, treatises, reviews, patents and monographs.

UNIT - II : CHEMICAL ABSTRACTS: (12 Hours)

Current awareness searching: CA weekly issues, CA issue indexes. Retrospective searching: CA volume indexes-general subject index, chemical substance index-formula index, index of ring systems, author index, patent index. CA collective indexes: collective index (CI), decennial index (DI). Access points for searching CA indexes- Index guide, general subject, terms, chemical substance names, molecular formulas, ring systems, author names, patent numbers. Locating the reference: finding the abstract, finding the original document chemical abstract - service source index.

UNIT –III: CHOOSING A RESEARCH PROBLEM AND SCIENTIFIC WRITING (12 Hours)

Identification of research problem – assessing the status of the problem - guidance from the supervisor – actual investigation and analysis of experimental results – conclusions.

Scientific writing-research reports, thesis, journal articles and books.

Steps to publishing a scientific article in a journal – types of publications-communications, articles, reviews, when to publish, where to publish ,specific format required for submission.

Documenting- Abstracts-indicative (or) descriptive abstracts, informative abstract, footnotes, end notes, referencing styles-bibliography-journal abbreviations (CASSI), abbreviation used in scientific writing.

Unit –IV: INSTRUMENTAL CHARACTERIZATION AND DATA ANALYSIS (12 Hours)

Principle and Sample preparation of UV, FT-IR, TEM, SEM, EDAX, AFM and XRD characterization of observed results – Data analysis - Report.

Errors in chemical analysis – classification of errors – determination of accuracy of methods – improving accuracy of analysis – significant figures – mean, standard deviation – comparison of results : "t" test, "f" test, Q test and "chi" square test – rejection of results – presentation of data.

UNIT –V: COMPUTER SEARCHES AND LITERATURE. (12 Hours)

ASAP – Alerts, CA Alerts, scifinder, chemport, science direct, STN international, journal home pages. Online browsing of research articles – online submission of research papers in various Journals (ACS, RSC, Elsevier, Springer etc.) –Instructions to the authors – Impact factors. Writing project proposal to funding agencies (UGC, DST etc.).

REFERENCES

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10. J.Gibaldi, W. S. Achtert, Handbook for writers of Research Papers; 2nd ed.; Wiley Eastern, 1987.
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12. http://www.dst.gov.in/whats_new/whats_new07/tsd-format.pdf
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14. R.M. Silverstein, G.C. Bassler and Morril, Spectrometric identification of organic compounds.
15. D.L.Pavia, G.M.Lampman and G.S.Kniz Jr., Introduction to spectroscopy – A guide for students of organic chemistry.
16. H.Willard, L.MerritJr.andA.Dean, Instrumental methods of analysis.
17. D.A.Skoog and M.West, Principles of instrumental analysis.
18. B.K.Sharma, Instrumental methods of chemical analysis.

19. D.A. Skoog and M.West, Fundamentals of analytical chemistry.
20. J.D.Dick, Analytical chemistry.
21. S.M.Khopkar, Basic concepts of analytical chemistry.

Organic Chemistry Practical – III

L T P C

0 0 4 2

Estimations, two stage preparations and Spectral interpretation have been included as the practical components.

Microscale preparations are recommended for the simple reason, they are both economic-friendly and eco-friendly

A.List of Estimations

1.Ethylmethylketone

2.Acetone

3. Saponification value of an oil

4.Determination of Percentage purity in an unsaturated acid.

5. Estimation of hydroxyl group

B. List of Two stage preparations

1.Benzaldehyde Benzoic acid m-nitro benzoic acid

2. Acetanilide p-acetanilide p-Bromoaniline

3.Methyl benzoate m-nitro methyl benzoate m-nitro benzoic acid

4. Acetanilide p-nitroacetanilide p - nitroaniline

5. Benzophenone Benzo phenone oxime Benzanilide

Students are expected to submit the recrystallised samples of the final products, at the time of practical examination, for evaluation by the examiners.

C. For Class work Only :

1. Download the following spectra from **internet** and give interpretation.
   Differentiate the following pair by H^1NMR spectra
   (a) Maleic acid and Fumaric acid.
   (b) Aqueous ethyl alcohol and Pure ethyl alcohol.

(c) Dimethyl Ether and Aqueous ethyl alcohol.

Interprete the following C-13 NMR Spectra.

(a)OFF- Resonance decoupled C-13 spectrum of menthol.

(b) DEPT spectrum of isopentyl acetate.

(c) INADEQUATE spectrum of 2- butanone.

Interprete the mass spectrum of anisole and benzoic acid.

N.B: 1.Section -C is course work only.

2. It is for the purpose of internal assessment only.

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INORGANIC CHEMISTRY PRACTICAL – III

L T P C
0 0 4 2

I. Quantitative estimation of a mixture containing two metal ions (Volumetric and Gravimetric Estimations).

1. Estimation of mixture of Cu^{2+} and Ni^{2+} ions.
2. Estimation of mixture of $Cu^{2+}$and Zn^{2+} ions.
3. Estimation of mixture of $Fe^{2+}$and Cu^{2+} ions.
4. Estimation of mixture of Fe^{2+} and Ni^{2+} ions.
5. Estimation of mixture of Ca^{2+} and Mg^{2+}ions.
6. Estimation of mixture of Ca^{2+} and Ba^{2+} ions.

II. Analysis of ores and alloys (course work).

III. One day visit to Industry/Research Institution and submission of a minor report.

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1. G.H. Jeffery, J. Bassett, J. Mendham and R.C. Denney, Vogel's *Textbook of Quantitative Chemical Analysis*, Revised 5th edition, ELBS, 1989.
2. Mounir A. Malati, *Experimental Inorganic/Physical Chemistry - An Investigative, Integrated Approach to Practical Project Work*, Woodhead Publishing Limited, Reprint 2010.

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PHYSICAL CHEMISTRY PRACTICAL-III

Objective: L T P C

0 0 4 2

To learn and apply the Principles of Potentiometric Titrations.

To understand the Principles and applications of Adsorption

I. POTENTIOMETRIC TITRATIONS

(a) Acid alkali titrations.

(b) Redox titrations (i) Fe^{2+} vs $Cr_2O_7^{2-}$

(d) Determination of dissociation constant of weak acids.

(e) Determination of activity and activity coefficient of ions.

(f) Determination of pH of a buffer solution using a quinhydrone electrode.

II. TITRATION USING PH METER

(a) Determination of dissociation constant of Weak acid.

III. ADSORPTION

Freundlich Adsorption isotherm

Adsorption of oxalic acid on charcoal.

REFERENCES

1. J.B.Yadav, " Advanced Practical Physical chemistry", 20th Edn., GOEL publishing House, Krishna Pakashan Media Ltd., (2001).
2. Findlay's "Practical Physical Chemistry" Revised and edited by B.P. Levitt 9th Edn., Longman, London, 1985.
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ORGANIC CHEMISTRY – IV

Objectives:

L T P C
4 0 0 4

To study the intermediate reactions, conformational, synthetic analysis, important Reagents in organic synthesis and the Steroid compounds.

Unit-I : Reaction under Intermediate chemistry (12 Hours)

Reaction Under Carbanion Intermediate: Stobbe, Darzen, acyloin condensation Shapiro reaction and Julia olefination.

Reaction through carbene intermediate: Bamford – Stevens , Reimer- Tiemann reactions.

Reaction Under Carbocation intermediate: Oxymercuration, halolactonisation, Baeyer-villiger oxidation

Reaction following Radical intermediate: Mc Murray coupling, Gomberg-Pechmann and Pschorr reactions.

Reaction involving Ylide intermediate: Wittig reaction and Peterson olefination.

Unit-II : Conformational analysis (12 Hours)

Conformation and configuration-conformational free energy-conformational analysis of mono substituted (alkyl, halogens) and 1,1-disubstituted (alkyl) and 1,2-1,3-and 1,4-dimethyl substituted cyclohexanes -compounds existing in boat form-conformation of cyclohexanone, decalin and perhydrophenanthrene-Curtin-Hammett principle- conformation and reactivity of acyclic and cyclic compounds (6membered).

Unit-III : Reterosynthetic analysis (12 Hours)

Synthon-synthetic equivalent-Functional group interconversions -use of protecting groups for alcohols, amines, acids, carbonyl compounds- use of activating and blocking groups-Robinson annulations reaction-carbon skeletal complexity-Role of key intermediates in organic synthesis. Reterosynthetic analysis of the following compounds: Twistane, cis - Jasmone, Baclofen, Trihexyl phenydyl, S-propanediol, Isonootkatone, cascarillic acid, camphor and 2,4-dimethyl-2-hydroxy pentanoic acid.

Unit-IV : Reagents in organic synthesis (12 Hours)

2,3-Dichloro-5,6-dicyano-1,4-benzoquinone (DDQ), DMSO, Super hydrides- Dess-martin-periodinane-Osmium tetra oxide.

Modern Reagents: Introductory treatment of the application of silicon (Tri alkyl silyl halides, organo silanes), Boron (9 – BBN, borane, and alkyl borane), phosphorus (phosphoranes),

palladium(Still coupling, Suzuki Coupling, Heck and Negishi reactions) samarium(SmI_2), ruthenium(RuO_2,Ru-Binap Complex), platinum(PtO_2, Adam's Catalyst) reagents in organic synthesis.

Unit-V : Steroid (12 Hours)

Classification- structural elucidation of cholesterol, irradiated products of ergosterol. Conversion of cholesterol to androsterone, progesterone, testosterone, 5α- and 5 β-cholanic acid. Conversion of Oestrone to Oestriol, Oestrodiol and vice-versa. Conformational structure of cholestane and Coprostane. General study of Bile acids and Prostoglandins.

REFERENCES

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2. R.T. Morrison and R.N. Boyd,'Organic Chemistry' sixth Edition, Prentice Hall, 1994

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INORGANIC CHEMISTRY- IV

Objectives: L T P C

4 0 0 4

- *To study the applications of Mossbauer, photoelectron and nuclear quadrupole resonance spectroscopic techniques in inorganic systems.*
- *To study the applications of ORD and CD to determine absolute configuration of chelate complexes.*
- *To introduce bioinorganic chemistry and to study role of metalloporphrins and metalloenzymes in various biological processes.*
- *To give an insight into material science.*

UNIT - I : SPECTRAL METHODS TO THE STUDY OF INORGANIC COMPOUNDS – II (12 Hours)

Mossbauer spectroscopy : Principle – isomer shift (IS) – splitting of resonance lines: quadrupole splitting and magnetic hyperfine splitting. Applications: MB spectra of iron compounds/complexes – structural elucidation, π- bonding effect, determination of high spin and low spin, spin state crossover and cis–trans isomers – nature of the complexes – mixed valence complexes. Tin compounds: MB spectra of Sn(II) and Sn(IV) compounds, oxidation states of Sn in its different compounds. Applications in bioinorganic chemistry: oxy and deoxy- hemerythrin - catalase, peroxidases, Fe-S protein systems.

ORD AND CD - Optical isomerism in octahedral complexes – absolute configuration of chelate complexes from ORD and CD.

UNIT - II: SPECTRAL METHODS TO THE STUDY OF INORGANIC COMPOUNDS – III (12 Hours)

Photo electron spectroscopy: Theory – types of PES –origin of fine structures – adiabatic and vertical transitions – PE spectra of homonuclear diatomic molecules (N_2, O_2) – hetero nuclear diatomic molecule (CO) – polyatomic molecules (H_2O, CO_2, CH_4, NH_3). Evaluation of vibrational constant – Koopman's theorem – application and limitation of the theorem. XPS (ESCA): structure of N_3^- ion, CCl_3CH_3, N (1s) spectrum of $[Co(en)_2(NO)_2]NO_3$, C(1s) spectrum of $C_2H_5COOCF_3$. Shake-up and shake-off processes – Structural and bonding information in metal carbonyls – Auger electron spectroscopy.

NQR spectroscopy: Applications – fingerprint technique. Investigating the electronic structure of molecules – information about EFG of nuclei – ionic character and hybridization of the bonds – structure of charge transfer complexes – Phase transition – hydrogen bonding.

Unit - III: BIOINORGANIC CHEMISTRY – I (12 Hours)

Non-metals and metals in biological systems, essential and trace elements; classification of metallo-biomolecules, coordination environment and entatic state. Metalloporphyrins – chlorophyll and photosynthesis; cytochromes, hemoglobin, myoglobin and dioxygen binding, vitamin B_{12} and co-enzyme – *in vivo* and *in vitro* nitrogen fixation. Iron storage and transport: ferritin, transferrins and siderophores, iron proteins: hemerythrin, cytochrome P450 enzyme, ferredoxin and rubredoxin.

Unit - IV: BIOINORGANIC CHEMISTRY – II (12 Hours)

Copper proteins and Enzymes : plastocyanin, azurin, hemocyanin and ascorbic oxidase – different types of Cu present in proteins and enzymes. Zinc enzymes: carboxypeptidase A, carbonic anhydrase and superoxide dismutase. Inhibition and poisoning of enzymes illustrated by xanthine oxidase and aldehyde oxidase. Toxicity of metals and the role of metallothionins – excess and deficient levels of Cu and Fe and the consequent diseases – chelate therapy – metal complexes as drugs, anticancer and antiarthritic agents. Metal complexes as probes of nucleic acids.

UNIT – V : CHEMISTRY OF INORGANIC MATERIALS (12 Hours)

Synthesis of inorganic materials – High temperature ceramic methods – Co-Precipitation and Precursor Methods – Combustion synthesis – High temperature reactions – precipitation, gel, solution and hydrothermal methods – Synthesis in sealed tubes and special atmospheres – Low temperature methods – Chemical Vapour Deposition (CVD) – Preparing single crystals -Epitaxy methods – Chemical Vapour Transport - Solution Methods. Insertion compounds of metal oxides – Intercalation compounds of graphite and transition metal disulphides. Zeolites: structures and properties – pillared clays – fullerenes and fullerides.

REFERENCES

1. Russell S. Drago, *Physical Methods in Inorganic Chemistry*, Chapman and Hall Ltd., London, 1965.
2. Russell S. Drago, *Physical Methods for Chemists*, Surfside Scientific Publishers, 2nd Edition, 1977.
3. E.A.V. Ebsworth, D.W.H. Rankin and S.Cradock, *Structural Methods in Inorganic Chemistry*, ELBS, 1988.
4. B.P.Straughan and S.Walker, *Spectroscopy* Volume 3, John Wiley and Sons Inc., Newyork, 1976.
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PHYSICAL CHEMISTRY- IV

Objective:

L T P C
4 0 0 4

- *To understand the Principles and applications of Vibrational and Raman spectroscopy*
- *To obtain Knowledge Fast reaction study*
- *To learn the Theories and applications of Kinetics*
- *To Know the Principles of Surface Chemistry and Catalysis*

UNIT - I: Vibrational Spectroscopy (12 Hours)

Vibrating diatomic molecule: Energy of diatomic molecules as simple harmonic oscillator-energy levels, vibrational transitions, selection rules; anharmonic oscillator-energy levels, selection rules, vibrational transitions. Diatomic vibrating rotator: Born-Oppenheimer approximation, vibration-rotation spectra, selection rules, P, Q, R branches. Vibrations of polyatomic molecules: symmetry and fundamental vibrations, normal modes of vibration, overtones, combination, difference bands; influence of rotations on the spectra of polyatomic molecules-parallel and perpendicular vibrations in linear and symmetric top molecules.

UNIT-II: Raman Spectroscopy (12 Hours)

Lasers: Nature of stimulated emission-coherence and monochromaticity, population inversion, cavity and mode characteristics, Q-switching, mode locking; types of lasers-solid-state, gas, chemical, and dye lasers.

Raman Effect: Quantum theory of Raman effect, Classical theory of Raman effect, Pure rotational Raman spectra- linear molecules, symmetric top and spherical top molecules, Vibrational Raman spectra-symmetry and Raman active vibrations, rule of mutual exclusion; Overtone and combination vibrations, Vibrational Raman spectra, Rotational Fine structure. Polarisation of light and Raman effect-The nature of Polarized effect, Vibrations of spherical top molecules and other types of molecules. Structure determination from Raman and Infra-red spectroscopy, Applications of IR and Raman spectroscopy: skeletal and group vibrations, finger printing and absorption frequencies of functional groups for inorganic and organic compounds. Techniques and instrumentation, Near-Infra-red FT-Raman spectroscopy.

UNIT-III: Chemical Kinetics I (12 Hours)

Reactions in Flow systems-Techniques for very fast reactions-Stopped-Flow method, Relaxation methods, Shock-Tube methods, Temperature, Pressure, electric field and magnetic field jump methods, Flash photolysis and pulse radiolysis. NMR and ESR methods of studying fast reactions.

Collision theory. Potential Energy surfaces-energy of activation. Statistical mechanics and chemical equilibrium- Derivations of rate equations Symmetry numbers and statistical factors. Application of ARRT to Reaction between atoms and reaction between molecules. Thermodynamic Formulation of conventional transition state theory, Limitations of transition state theory. Vibrational transition state theory, Quantum mechanical transition state theory , Microscopic reversibility. Unimolecular reactions- Lindemann-Christiansen hypothesis, Hinshelwood, RRK, RRKM and Slater theories.

UNIT-IV: Chemical Kinetics II (12 Hours)

Elementary reactions in solution-Solvent effects on reaction rates, Factors determining reaction rates in solution- collisions in solution, Transition State Theory, Influence of internal pressure, influence of salvation. Reaction between ions- Influence of solvent dielectric constant, Pre-exponential Factors, Single-Sphere Activated Complex, Influence of ionic strength. Influence of Hydrostatic Pressure-Van't Hoff's equation and volumes of activation. Substituent and correlation effects-Hammett equation, Compensation effect.

Composite reactions-Types of composite mechanism, Rate equations for composite mechanisms, Simultaneous and consecutive reactions, Steady –State Treatment, Kinetics of H_2-Cl_2 and H_2-Br_2 reactions, Formation of Phosgene-decomposition of O_3 and N_2O_5. Rice-Herzfeld mechanism, Explosive reactions: H_2-O_2 reaction.

UNIT-V: Surface Chemistry & Catalysis (12 Hours)

Introduction: Adsorption- Physisorption and chemisorptions. Adsorption isotherms: Freundlich, Langmuir, BET and Gibbs adsorption isotherms. Surface area dertermination. ARRT to surface reactions. Micelles: Micelles and reverse micelles- microemulsion-solubilisation.

Catalysis: Homogeneous catalysis- acid-base catalysis- Van't Hoff and Arrehenius complexes for Protropic and Protolytic mechanisms. Bronsted catalysis law- Hammett acidity function. Heterogeneous catalysis. Chemical reactions on solid surfaces. Enzyme catalysis: Michaelis-Menton Kinetics- Rate of enzyme catalyzed reaction- effect of substrate concentration, pH and temperature on enzyme catalyzed reactions.

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Organic Chemistry Practical – IV

L T P C
0 0 4 2

Estimation, two stage preparations and chromatographic techniques have been included as the practical components.

Microscale preparations are recommended for the simple reason, they are both economic-friendly and eco-friendly

A.List of Estimation

1.Glucose-Lane Eynon and method

2.Glucose-Bertrand's method

3.Iodine value of an oil

4. Estimation of acetyl group

5. Purity of Glucose.

B. List of Two stage preparations

1. Benzophenone Benzpinacol Benzpinacolone

2. Phthalic acid Phthalic anhydride Phthalimide

3. Thiourea s-benzyl isothiuronium chloride s- Benzyl-isothiuronium benzoate

4. Aniline Tri-bromoaniline Sym- Tribromobenzene

5.Phthalic anhydride ⟶ Phthalimide ⟶ Anthranilic acid

Students are expected to submit the recrystallised samples of the final products, at the time of practical examination, for evaluation by the examiners.

For Class work Only .

1. Isolation of carotene from carrot.
2.

REFERENCES

1.F.C.Mann and B.C.Saunders, Practical organic chemistry, Fourth edition, ELBS,1970

2.A.I. Vogel, A Text book of Practical organic chemistry.

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INORGANIC CHEMISTRY – IV

L T P C
0 0 4 2

I. Preparation of inorganic complexes and quantitative estimation by volumetric or instrumental methods.

1. Preparation, and analysis of potassium trisoxalatochromate(III) trihydrate $K_3[Cr(C_2O_4)_3].3H_2O$
2. Preparation and analysis of potassium hexathiocyanatochromate(III) tetrahydrate $K_3[Cr(SCN)_6].4H_2O$
3. Preparation and analysispotassium trisoxalatomanganate(III) trihydrate $K_3[Mn(C_2O_4)_3].3H_2O$
4. Preparationand analysis of potassium trisoxalatoferrate(III) trihydrate $K_3[Fe(C_2O_4)_3].3H_2O$
5. Preparation and analysis of potassium trisoxalatocobaltate(III) trihydrate, $K_3[Co(C_2O_4)_3].3H_2O$
6. Preparation and analysis of Durrant's salt, $K_4[C_2O_4)_2Co(OH)_2Co(C_2O_4)_2].3H_2O$
7. Preparation and analysishexamminecobalt(III) Chloride, $[Co(NH_3)_6]Cl_3$
8. Preparation and analysis of chloropentaamminecobalt(III) chloride, $[Co(NH_3)_5Cl]Cl_2$
9. Preparation and analysis of trinitrotriamminecobalt(III), $[Co(NH_3)_3(NO_2)_3]$
10. Preparation and analysis of trans-dichlorobis(diaminoethane)cobalt(III) chloride, trans-$[Co(en)_2Cl_2]Cl$
11. Preparation and analysis of $(NH_4)_2[VO(C_2O_4)_2].2H_2O$
12. Preparation and analysis of tris(thiourea)copper(I) sulphate dihydrate, $[Cu(tu)_3]_2SO_4.2H_2O$

II. Characterisation of metal complexes prepared during the practicals by UV and IR spectral techniques (Course work).

III. Study of linkage isomerism in pentaamminenitritocobalt(III) chloride, and pentaamminenitrocobalt(III) chloride using IR (Course work).

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1. Mounir A. Malati, *Experimental Inorganic/Physical Chemistry - An Investigative, Integrated Approach to Practical Project Work*, Woodhead Publishing Limited, Reprint 2010.
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5. Geoffrey Pass, Haydn Sutcliffe, *Practical Inorganic Chemistry - Preparations, reactions and instrumental methods*, Springer 1974.

PHYSICAL CHEMISTRY PRACTICAL-IV

Objective: L T P C

0 0 4 2

To obtain and improve the Knowledge of Potentiometric Titrations.

To understand the Principles and applications of Adsorption

POTENTIOMETRIC TITRATIONS

I. **Precipitation titrations**

Mixture of Cl^- and I^- vs Ag^+

II. **Redox titrations**

(i) Fe^{2+} vs Ce^{4+}

(ii) I^- vs $KMnO_4$

III. **Solubility Product** Determination of solubility product of sparingly soluble silver salts.

ADSORPTION

Freundlich Adsorption isotherm:

Adsorption of acetic acid on charcoal.

REFERENCE BOOKS (Practical I to IV)

1. J.B.Yadav, " Advanced Practical Physical chemistry", 20th Edn., GOEL publishing House, Krishna Pakashan Media Ltd., (2001).
2. Findlay's "Practical Physical Chemistry" Revised and edited by B.P. Levitt 9th Edn., Longman, London, 1985.
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Project