## **SYLLABUS**

## MANONMANIAM SUNDARANAR UNIVERISTY, TIRUNELVELI-12

## PG - COURSES - AFFILIATED COLLEGES

Course Structure for

# M.Sc. Chemistry

( Choice Based Credit System)

( with effect from the academic year 2017- 2018 onwards )

| Semester-III |                   |                                     |                 |        |
|--------------|-------------------|-------------------------------------|-----------------|--------|
| Part         | Subject<br>Status | Subject Title                       | Subject<br>Code | Credit |
| 3            | Core              | Organic Chemistry – III             | PCHM31          | 4      |
| 3            | Core              | Inorganic Chemistry – III           | PCHM32          | 4      |
| 3            | Core              | Physical Chemistry – III            | PCHM33          | 4      |
| 3            | Core              | Scientific - Research Methodology   | PCHM34          | 4      |
| 3            | Practical         | Organic Chemistry Practical – III   | PCHL31          | 2      |
| 3            | Practical         | Inorganic Chemistry Practical – III | PCHL32          | 2      |
| 3            | Practical         | Physical Chemistry Practical – III  | PCHL33          | 2      |

## ORGANIC CHEMISTRY – III

#### **Objectives:**

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

#### Unit-I

#### Aliphatic nucleophilic substitution and Elimination Reactions:

Aliphatic nucleophilic substitution: Mechanism of  $S_N1$ ,  $S_N2$ ,  $S_Ni$ ,  $S_N1$ ,  $S_N2$  and SNi 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**

<sup>1</sup>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<sup>1</sup>NMR - chemical shifts (aliphatic, olefinic, alkynic, aromatic and carbonyl compounds)

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

#### Unit – III:

#### MASS SPECTROSCOPY

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, H1 NMR, 13C 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

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- $\pi$  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**

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.

- 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
- 4. Inc., Singapore, 2006.
- 5. Raj K. Bansal, 'Organic Reaction mechanisms', Tata Mc Graw Hill, Third Editon, 2007
- 6. Singh, J., and Singh, J., "Photochemistry and Pericyclic reaction", New Age International, New Delhi, 2004
- 7. H.O. House, 'Modern synthetic Reaction,' Second Edition, W.A. Benjamin, Inc., London, 1972
- 8. R.K. Mackie, M.M. Smith and R.A. Aitken, 'Guide Book to Organic Synthesis' Second Edition, Longman Seientific and Technical, Singapore, 1990.
- 9. Carrutherus, W., "Some Modern Methods in Organic Syntheis", Third edition, Cambridge University Press, New York, 1997.
- 10. F.A. Carey and J.Sundberg, 'Advanced Organic chemistry ' part A and B, Plenum Press, 2005.
- 11. Michael B. Smith, 'Organic Synthesis,' Mc Graw Hill international Edition ,1994
- 12. P. Sykes, 'A Guide book to mechanism in organic chemistry', Orient Longman, 1989.
- 13. Gurdeep R. Chatwal, 'Reaction mechanism and Reagents in organic



- chemistry', Himalaya publishing House, Bombay 1992.
- 14. R.T. Morrison and R.N. Boyd, 'Organic Chemistry' sixth Edition, Prentice Hall, 1994
- 15. R.O.C .Norman, Principles of organic synthesis- Chapman and hall, London.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, 5<sup>th</sup> 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
- 20. Bansal, K., "Heterocyclic Chemistry", Fourth edition, New Age International, New Delhi, 2005.

## **INORGANIC CHEMISTRY - III**

### **Objectives:**

- 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

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

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 mechanism stereoregular and of 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

**NMR SPECTROSCOPY:** <sup>31</sup>P, <sup>19</sup>F and <sup>15</sup>N – NMR – applications in structural problems based on number of signals, multiplicity, anisotropy (like H<sub>3</sub>PO<sub>3</sub>, H<sub>3</sub>PO<sub>2</sub>, [HNi(<sub>PPh3</sub>)4]+, SF<sub>4</sub>, TiF<sub>4</sub>, PF<sub>5</sub>, HPF<sub>2</sub>, H<sub>2</sub>PF<sub>3</sub>, PF<sub>3</sub>(NH<sub>2</sub>)<sub>2</sub>, P<sub>4</sub>S<sub>3</sub>, P<sub>4</sub>N<sub>4</sub>Cl<sub>6</sub>(NHC<sub>6</sub>H<sub>5</sub>)<sub>2</sub>, P<sub>3</sub>N<sub>3</sub>(CH<sub>3</sub>)2C<sub>14</sub>, NF<sub>3</sub>, NH<sub>3</sub> – mer- and fac-Rh(PPh<sub>3</sub>)<sub>3</sub>C<sub>31</sub>, 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<sub>2</sub>],  $[(NH_3)_5Co-O_2 Co(NH_3)_5]_{5+}$ Co<sub>3</sub>(CO)<sub>9</sub>Se, Co<sub>3</sub>(CO)<sub>9</sub>Rh,  $[CrF_6]3-,$  $VO(acac)_2$ ,  $[CoF_6]_{4}$ -, [VO(H<sub>2</sub>O)<sub>6</sub>]<sub>2</sub>+, [Fe(CN)<sub>5</sub>NO]<sub>2</sub>-). 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

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

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.

- 1. James E. Huheey, Ellen A. Keiter and Richard L. Keiter, Inorganic Chemistry, Principles of Structure and Reactivity, 4th Edition, Harper Collins College Publishers, 1993.
- 2. F. Albert Cotton, Geoffrey Wilkinson, Carlos A. Manic and Manfred Bochman, Advanced Inorganic Chemistry, Wiley Interscience Publication, 6th Edition, 1999.
- 3. D.F. Shriver, P.W. Atkins and C.H. Langford, Inorganic Chemistry, ELBS, Oxford University Press, 1994.
- 4. R. H. Crabtree, The Organometallic Chemistry of the Transition Metals, 4th Edition, John Wiley, 2005.
- 5. C. Elschenbroich, A. Salzer, Organometallics A Concise Introduction, 2nd Edition, VCH Publication, 1992.
- 6. R. C. Mehrotra, A. Singh, Organometallic Chemistry: A Unified Approach,



- 2nd Edition, New Age International, 2000.
- 7. K.F. Purcell and J.C. Kotz, Advanced Inorganic Chemistry, Saunders Golden Publishers, 1977.
- 8. B.E. Douglas, D.H. McDaniel and J.J. Alexander, Concepts and Models of Inorganic Chemistry, John Wiley and Sons Ltd., 2nd Edition, 1983.
- 9. Russell S. Drago, Physical Methods in Inorganic Chemistry, Chapman and Hall Ltd., London, 1965.
- 10. Russell S. Drago, Physical Methods for Chemists, Surfside Scientific Publishers, 2nd Edition, 1977.
- 11. E.A.V. Ebsworth, David W.H. Rankin, Stephen Credock, Structural Methods in Inorganic Chemistry, ELBS, 1988.
- 12. David W. H. Rankin, Norbert W. Mitzel, Carole A. Morrison, Structural Methods in Molecular Inorganic Chemistry, John Wiley & Sons, Ltd, 1st Edition, 2013.
- 13. Robert A. Scott and Charles M. Lukehart, Applications of Physical Methods to Inorganic and Bioinorganic chemistry, John Wiley & Sons Ltd, 2007.
- 14. Philip H Rieger, Electron Spin Resonance Analysis and Interpretation, The Royal Society of Chemistry, 2007.
- 15. John A. Weil, James R. Bolton, Electron Paramagnetic Resonance Elementary Theory and Practical Applications, 2nd Edition, John Wiley & Sons, 2007.
- 16. D.A. Skoog, F.J. Holler and T.A. Nieman, Principles of Instrumental Analysis, Saunders, 1992.
- 17.D.A. Skoog, D. M. West, F.J. Holler, S.R. Grouch, Fundamentals of Analytical Chemistry, Thomson Asia Pvt.Ltd., 8th Edition, Third Reprint, 2005.
- 18. H.H. Willard, L.L. Merritt and J.A. Dean, Instrumental Methods of Analysis, CBS Publishers, 6th Edition, 1986.
- 19. D. M. Roundhill, Photochemistry and Photophysics of Metal Complexes, Plenum Press, 1990.
- 20. A.W. Adamson and P.D. Fleischauer, Concepts of Inorganic Photochemistry, John wiley and sons, New York, 1975.
- 21. Journal Chemical Education, Vol. 60, No.10, 1983.
- 22. K. Kalyanasundaram, Photochemistry of polypyridine and phorphyrin complexes, Academic Press, London, 1992.
- 23. V. Balzani, F.Bolletta, M. Ciano and M.Maestry, J.Chem. Edu., Vol. 60, 447, 1983.
- 24. V. Balzani and A.Juris, Coord. Chem. Rev., 211, 97–115, 2001.

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## PHYSICAL CHEMISTRY- III

## **Objective:**

- Learning the concepts of Group Theory
- To understand the Principles and applications of various spectroscopy

#### **UNIT-I:**

## **Group Theory-I**

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:**

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**

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 <sup>13</sup>C, <sup>19</sup>F, <sup>31</sup>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 OverhauserEffect (NOE), 2D NMR-shift correlation spectra-COSY, Magnetic Resonance Imaging (MRI).

#### **UNIT-IV:**

NQR and EPR spectroscopy



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

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.
- 10. K. V. Raman, R. Gopalan and P. S. Raghavan, Molecular Spectroscopy, Thomson and Vijay Nicole, Singapore, 2004.



- 11. I.N. Levine, Molecular Spectroscopy, John Wiley & Sons, New York, 1974.
- 12. Organic spectroscopy, William Kemp, Third Edition.
- 13. Spectroscopy (Atomic and Molecular) Gurdeep R. Chatwal and Sham K. Anand, Himalaya Publishing House
- 14. R. S. Drago, Physical Methods in Chemistry; Saunders: Philadelphia, 1977.
- 15. J. A. Weil, J. R. Bolton and J. E. Wertz, Electron Paramagnetic Resonance; Wiley Interscience: 1994.
- 16. Introduction to Molecular spectroscopy, G.M. Barrow, McGraw-Hill international editions.
- 17. R.M.Silverstein and F. X. Webster, Spectroscopic Identification of Organic Compounds, 6th ed., John Wiley & Sons, New York, 2003.

## SCIENTIFIC - RESEARCH METHODOLOGY

## **Objectives:**

- 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

Source of chemical information – primary, secondary, tertiary sourcesliterature 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:**

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

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

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

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.).

- 1. R.T. Bottle, The use of Chemical literature, Butterworths, 1969.
- 2. A.J. Durston, Thesis and assignment writing.
- 3. R.O.Bullet, Preparing thesis and other manuscripts.
- 4. R. L. Dominoswki, Research Methods, Prentice Hall, 1981.
- 5. J. W.Best, Research in Education, 4th ed. Prentice Hall of India, New Delhi, 1981.
- 6. H. F. Ebel, C. Bliefert and W. E. Russey, The Art of Scientific Writing, VCH, Weinheim, 1988.
- 7. B. E. Cain, The Basis of Technical Communicating, ACS., Washington, D.C., 1988.
- 8. H. M. Kanare, Writing the Laboratory Notebook; American Chemical Society: Washington, DC, 1985.
- 9. J. S. Dodd, Ed., The ACS Style Guide: A Manual for Authors and Editors; American Chemical Society: Washington, DC,1985.
- 10. J.Gibaldi, W. S. Achtert, Handbook for writers of Research Papers; 2nd ed.; Wiley Eastern, 1987.
- 11. Joseph, A. Methodology for Research; Theological Publications: Bangalore, 1986.
- 12. http://www.dst.gov.in/whats\_new/whats\_new07/tsd-format.pdf
- 13. www.ugc.ac.in/pdfnews/7716504\_12th-plan-guidelines.pdf
- 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. Merrit Jr. and A. 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**

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-nitro acetanilide 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 H1NMR 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.

- 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.
- 3. A.I. Vogel, A Text book of Quantitative Organic Analysis, 1989.
- 4. Raj K. Bansal, Laboratory Manual of Organic Chemistry, Second Edition, Wiley Eastern Ltd., 1990



- 5. Moore, Dalrympk and Rodig, Experimental methods in organic chemistry, 3rd edition, Saunders College publishing, The Oxford Press,1982
- 6. Bassett et.al., A Text Book of Quantitative Inorganic Analysis, ELBS, 1986
- 7. Roberts, Gilbert, Reidwald-Wingrove An Introduction to Experimental Organic Chemistry, 1969.
- 8. V.K.Srivastava and K.K.Srivastava, Introduction to Chromatography-Theory and Practice, S.Chand & Co., 1987.

## INORGANIC CHEMISTRY PRACTICAL – III

- I. Quantitative estimation of a mixture containing two metal ions (Volumetric and Gravimetric Estimations).
- 1. Estimation of mixture of Cu2+ and Ni2+ ions.
- 2. Estimation of mixture of Cu2+and Zn2+ ions.
- 3. Estimation of mixture of Fe2+and Cu2+ ions.
- 4. Estimation of mixture of Fe2+ and Ni2+ ions.
- 5. Estimation of mixture of Ca2+ and Mg2+ions.
- 6. Estimation of mixture of Ca2+ and Ba2+ ions.
- II. Analysis of ores and alloys (course work).
- III. One day visit to Industry/Research Institution and submission of a minor report.

- 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



## PHYSICAL CHEMISTRY PRACTICAL-III

#### **Objective:**

- 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) Fe2+ vs Cr2O7 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.

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