MASTER OF PHILOSOPHY IN CHEMISTRY

SYLLABUS - 2007-09

ST. JOSEPH'S COLLEGE (AUTONOMOUS)

(Nationally Reaccredited with A+ Grade / College with Potential for Excellence)

TIRUCHIRAPPALLI - 620 002

TAMIL NADU, INDIA

ST. JOSEPH'S COLLEGE (AUTONOMOUS), TIRUCHIRAPPALLI - 620 002
DEGREE OF MASTER OF PHILOSOPHY (M. PHIL.)
FULL TIME - AUTONOMOUS REGULATIONS

GUIDELINES

1. ELIGIBILITY

✧ A Candidate who has qualified for the Master's Degree in any Faculty of this University or of any other University recognized by the University as equivalent there to (including old Regulations of any University) subject to such conditions as may be prescribed therefore shall be eligible to register for the Degree of Master of Philosophy (M.Phil.) and undergo the prescribed course of study in a Department concerned.

✧ A candidate who has qualified for Master's degree (through regular study / Distance Education mode / Open University System) with not less than 55% of marks in the concerned subject in any faculty of this university or any other university recognized by Bharathidasan University, shall be eligible to register for M.Phil. SC / ST candidates are exempted by 5% from the prescribed minimum marks.

2. DURATION

The duration of the M.Phil. course shall be of one year consisting of two semesters for the full-time programme.

3. COURSE OF STUDY

The course of study shall consist of

Part - I : 3 Written Papers
Part - II : 1 Written Paper and Dissertation.

The three papers under Part I shall be :

Paper I : Research Methodology
Paper II : Advanced / General Paper in the Subject
Paper III : Advanced Paper in the subject

Paper I to III shall be common to all candidates in a course. Paper I, II, III & IV shall consist of 5 units each covering the subject requirements of the course offered. The Board of Studies shall approve the Syllabi for Papers. The syllabus for paper IV shall be prescribed by each Research Advisor, which is also to be approved by the Board of Studies. The number of specialized papers by the research advisor can be more than one.

Question papers for Papers I to III shall be set externally and valued by two examiners, one internal and one external. The concerned HOD will be in the Board of Examiners to pass the results. Paper IV shall be set and valued by the Research Adviser. The Controller of Examinations shall conduct the examinations for all papers and dissertation.

4. SCHEME OF EXAMINATION

4.1 Part-I (First Semester)

Paper I : Research Methodology
Paper II : Advanced / General paper in the subject
Paper III : Advanced paper in the subject

Part-II (Second Semester)

Paper IV : Field of specialization
Paper V : Dissertation

4.2 Written Examination

The examinations for Papers-I, II and III shall be taken at the end of the first semester and Paper-IV at the end of the second semester. Each paper shall have 100 marks for the semester examination (written) and 100 marks for Continuous Internal Assessment.

The CIA components are:

Seminar-I	:	15 marks
Mid semester	:	35 marks
Seminar-II	:	15 marks
End semester	:	35 marks
Total	:	100 marks

Both the CIA marks and the external marks should be mentioned separately in the mark sheets. The duration for each semester examination shall be 3 hours. A candidate shall be declared to have passed Part-I & II examinations if he/she secures not less than 50 of the marks each in the CIA and the semester examination respectively. The aggregate of the marks secured in the semester examinations and CIA marks taken together must be 50% in each of the Papers I to IV and Dissertation.

4.3 Credits for Papers I to IV

Paper	Name	Contact Hours	Library Hours	Total Hours	Credits	CIA Marks
I	Research Methodology	6	6	12	10	100
II	Core Subject	6	6	12	10	100
III	Core Subject	6	6	12	10	100
IV	Optional Subject	2	4	6	5	100
	Total			42	35	400

Credits for Dissertation

Internal Examination (the split up for CIA)

Project	Credits	Marks	Total Marks
Seminar on review of related literature	3	30	200
Seminar on Data Analysis / Results	2	20	
Dissertation Evaluation	15	150	
Viva - voce	5	100	100
Total	**25**	**300**	**300**

External Examination

	Credits	Marks
Dissertation Evaluation	20	200
Viva-voce	5	100
Total	**25**	**300**

4.4 Dissertation

For carrying out the dissertation the mandatory requirement is strictly adhering to the rules of the college as given below:

4.4.1a Requirement

Every student is expected to give two seminars one concerning Review of Related Literature within the four weeks from the beginning of the second semester and the other on Data Analysis / Result just before the submission of the final draft of the dissertation

4.4.1b Submission

Candidates shall submit the Dissertations to the Controller of Examination not earlier than five months but within six months in the full time programme. The above said time limit shall start from 1st of the month which follows after the month in which Part-I examinations are conducted. If a candidate is not able to submit his/her Dissertation within the period stated above, he/she shall be given an extension time of three months in the first instance and another three months in the second instance with penalty fees. If a candidate does not submit his Dissertation even after the two extensions, his registration shall be treated as cancelled and he has to re-register for the course subject to the discretion of the Principal. However the candidate need not write once again the theory papers if he / she has already passed these papers.

4.4.1c Requirement

For the valuation of dissertation the mandatory requirement is a pass in papers I to IV. One external examiner and the Research Adviser shall value the Dissertation. The external examiner should be selected only from outside the college and shall be within the colleges affiliated to Bharathidasan University. In case of non-availability, the panel can include examiners from the other university / colleges in Tamil Nadu. The external examiner shall be selected from a panel of 3 experts suggested by the Research Adviser. However, the Controller of Examination may ask for another panel if he deems it necessary. Both the internal and external examiner will evaluate the Dissertation and allot the marks separately. However the viva-voce will be done by both of them. The average marks will be considered.

4.4.2 Viva-voce

The external examiner who valued the Dissertation and the Research Adviser shall conduct the Viva-Voce for the candidate for a maximum of 100 marks. A Candidate shall be declared to have passed in viva-voce if he secures not less than 50% of the marks prescribed for Dissertation and 50% of the marks in the aggregate of the marks secured in viva-voce test and Dissertation valuation. A student can undertake project in the second semester whether or not he /she has passed the first semester.

5. QUESTION PAPER PATTERN

5.1 Internal (Mid & End)

5.1a For Science

There are two sections A and B:

Section A contains 8 short answer Questions	8 × 4	= 32
Section B contains 4 Essay Question	4 × 17	= 68
		100

5.1b For Arts

Only one section of Essay type questions 5 × 20 = 100

5.2 External Exam (Semester)

5.2a For Science

Section A - 10 short answer Questions	10 × 3	= 30
Section B - 5 Essay type Questions either or	5 ×14	= 70
		100

5.2b For Arts

Only one section of Essay type questions 5 out of 8 (5 × 20 = 100)

5.2c For the Paper-IV (Optional/Research Adviser's paper)

The Question paper pattern for Paper IV is common for both Science and Arts. The pattern is only one section with Essay type Questions 5 out of 8 (5 × 20 = 100)

There may be two separate mark sheets for the first and second semester respectively. The marks allotted by the guide and that by the External Examiner must be shown in separate columns of the 2nd Semester mark sheet.

6. CLASSIFICATION OF SUCCESSFUL CANDIDATES

6.1 The candidates who pass the Part - I and Part - II examinations in their first attempt shall be classified as follows:

No.	Total Marks secured in Part - I and Part - II Examinations	Classification
1.	80% and above in the case of Science Subjects & 75% and above in the case of Arts and Social Science Subjects	I Class with Distinction
2.	60% to 79% in the case of Science Subjects & 60% to 74% in the case of Arts and Social Science Subjects	I Class
3.	50% to 59% in all the subjects (Mathematics, Statistics and Computer Science / Applications shall be treated as Science Subjects)	II Class

6.2 Candidates who pass the course in more than one attempt shall be declared to have completed the programme under II Class.

7. QUALIFICATIONS OF RESEARCH ADVISER FOR THE M.Phil. COURSE

7.1 A person eligible to be a Research Adviser shall be required to possess a Ph.D. Degree or two years of Post-Graduate teaching experience after qualifying for M.Phil. / M.Litt. degree. He / She should have obtained recognition from the University.

7.2 In view of the paucity of guides in the newly emerging subjects like Biotechnology, Microbiology, Remote Sensing the research guides in the related areas may be permitted to guide students provided these guides satisfy the qualification requirements.

7.3 Normally a person shall be allowed to guide not more than three candidates.

7.4 Change of guide may be permitted by the Principal based on the merit of the individual cases.

8. ATTENDANCE

- ✧ Daily attendance for 90 working days should be enforced for the students.
- ✧ Periodical report of a student to the guide concerned should be recorded in the register kept by the guide.

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M.PHIL. CHEMISTRY - COURSE PATTERN - 2007

Sem	Code	Course	Title of the paper
I	07 MCH 101	I	Research Methodology
	07 MCH 102	II	Physical Methods in Chemistry
	07 MCH 103	III	Recent Trends in Chemistry
II	07 MCH 204	IV	Thermodynamics & Physical Properties of Liquid Solution
	07 MCH 205	IV	Reactivity of Ether Linkage
	07 MCH 206	IV	Kinetics And Mechanism
	07 MCH 207	IV	Advanced Coordination Chemistry
	07 MCH 208	IV	Reactivity of Ether Linkage
	07 MCH 209	IV	Advanced Studies of Macrocyclic Complexes
	07 MCH 210	IV	Organic Reaction Mechanism
	07 MCH 211	IV	Physical Methods in Inorganic Chemistry
	07 MCH 212	IV	Corrosion Inhibition on Metals
	07 MCH 213	IV	Natural Products Chemistry
	07 MCH 214	IV	Advanced Coordination Chemistry
	07 MCH 215	IV	Thermodynamics of Liquid Solutions
	07 MCH 216	IV	Physical Methods in Inorganic Chemistry
	07 MCH 217	IV	Electro Organic Chemistry
	07 MCH 218	IV	Organic Synthesis
	07 MCH 219	IV	Organic Reaction Mechanism

Paper I : RESEARCH METHODOLOGY

Unit I: Information Retrieval & Documentation

Sources of information -Primary, secondary, tertiary Sources-Journals-Abstracts-Current Titles-Reviews-Monographs-Dictionaries-Information retrievals using internet and other electronic medias [Preparing a review Article related to the problem of Research of the student]. Reports of Research Work - Laboratory Observation- Preparation of Records-Manuscripts-Research Paper formats in Indian J.Chemistry., J.Indian Chem.Soc., J.Am.Chem.Soc. J.Chem.Soc., Tetrahedron. Anal.Chem. J.Chem. Education, etc, Writing of the project report or thesis. IUPAC nomenclature of Organic & Inorganic Compounds. IUPAC Nomenclature of organic and inorganic compounds.

Unit II Statistical Tools of research

Error Analysis- Errors-Types-Precision, and accuracy - Significant figures-Tests for accuracy of results-Positive and negative deviation from accuracy-Distributions: Binomial, Gaussian, etc.,- The normal distribution of random errors -mean value- Variance-standard deviation-reliability interval- t- test, F- test- Regression-standard deviation- Correlation coefficient-Multiple linear Regression- Observation, Inference- Hypothesis generation- Testing of Hypothesis-Evolving and modifying Rules & Theories.

Unit III: Computers in Chemistry

Introduction to computers- history of development of computers Main frame mini, micro and super computer systems-computer hard ware CPU, input, output devices, auxiliary storage devices, interpreter, compiler, machine language, assembly language, high level languages-Operating systems, MS Dos, windows, UNIX, basic ideas in LINUX -Languages- C Language & Programmeming- Constants, variables, function- Logical & Arithmetic statements- Transfer & control structure- array pointers-File handling procedures, simple programmeming examples from chemistry 'Temperature conversion, Calculation of frequency of electromagnetic Radiation, C_v of Solid (C_v at T< 30 K and at T > 30 K), Activity coefficient of Electrolytes, Rate constants of I & II order reactions, $t_{1/2}$ of I, II & III order reactions, Calculation of Arrhenius Parameters, Calculation of Modes of Vibration Introductory Operatives-Package, MS word, MS Excell, MS Power Point - Preparation of a document-Editing of a document-Preparing a scientific manuscripts - Features of Acrobat Reader.

Unit IV: Methods of organic synthesis

Synthons - nucleophiles - Electrophiles- Introduction of Functional Groups- Interconvertion of functional groups like C=O, -CHO, -OH, -SH, -COOH,-NH_2, -COOR, -CONHR, C=C . Protection of some functional groups Regio selective, Regio specific & stereo selective alkylation of cyclic Ketones & enones - C- alkylation- enamines and selective alkylation- O-alkylation - Olefination of Carbonyl compounds-Wittig reaction. Retro synthetic Analysis of simple organic compounds- mono & bi-functional open chain target molecules mono & bi-cyclic target molecules. Multi-step organic synthesis. Reduction- Catalytic hydrogenation-Dehydrogenation-use of NaH, $LiAlH_4$, Tri-tertiary butoxy Aluminium Hydride, $NaCNBH_3$, $SiMe_3H$, Alkali metal in Acidic, Basic, Neutral solvents, Hydrazines. Oxidation- OsO_4, CrO_2Cl_2, O_3, HIO_4, Dioxane, lead tetra acetate, SeO_2, Microwave assisted reactions.

Unit V: Methods of separation

Extraction- Solvent extraction principle -Theory- Different methods of extraction-separation techniques-chromatography- Paper, thin layer, Column Chromatography- Ion-exchange chromatography-GC and HPLC techniques-GC-MS Techniques-Principles and uses of other separation techniques: Filtration- Crystallisation.

Text Books

1. March J, 1996, "Advanced Organic Chemistry Reactions, Mechanisms and Structure." 5th ed, New York, Wiley.
2. Drago R.S., 1971, "Physical Methods in Inorganic Chemistry", 3rd ed., New Delhi, Wiley Eastern Company.
3. Banwell C.N., 1983, "Fundamentals of Molecular Spectroscopy", 3rd ed., New Delhi.Mc Graw Hill.
4. Kemp W, 1993, Organic Spectroscopy, 3rd edition, London, ELBS with Macmillan.
5. Raman K.V., 1993, "Computers in chemistry",1st ed, New Delhi, Tata Mc Graw Hill,.

References

1. Silverstein and webstr: 1998, "Spectrometric identification of Organic Compounds", sixth Edition, New York, Wiley.
2. Vogel A. I., 1961, "Quantitative Inorganic Analysis". 3rd ED., London ELBS Longman.
3. Pine S.H., Hendrickson J.B., Cram D.J. and Hammond G.S., 1980, "Organic Chemistry," 4th ed, Mc Graw Hill.
4. Lowry T.H. and Richardson K.S., 1976, "Mechanism and Theory in Organic Chemistry", Harper and Row.
5. Adamson A.W., "Physical Chemistry of Surfaces", 4th ed., John Wiley.
6. Trapnell B.M.W., 1955, "Chemisorptions", New York, Academic Press,.
7. Drago R.S., 1992, "Physical Methods in Chemistry", 3rd ed, Philadelphia, London, W.B. Saunders Company.
8. Wheatly P.J., 1959, "The Determination of Molecular Structure", London, Oxford at the Clarendon Press.
9. Ebsworth E.A.V., 1987 "Structural Methods in Inorganic Chemistry", 3rd ed, Great Britain, ELBS.
10. Gibbs T.C., 1976 "Principles of Mossbauer Spectroscopy," London, Chapman and Hall.
11. Barrow G., 1964, "Introduction to Molecular Spectroscopy,"2nd ed, NY, McGraw Hill.
12. Ghosh P.K., 1989, "Introduction to Photoelectron Spectroscopy," New York, John Wiley.
13. Becker C.D., 1980, "High Resolution NMR-Theory and Applications", 2nd ed., London, Academic Press.
14. Straughan B. P. and Walker S. 1976, "Spectroscopy Vol 1", London, Chapman & Hall,.
15. Eckschlager K., 1969, "Errors, Measurement and results in chemical analysis", London, Van Nostrant Reinhold company, chapters-I, IV, V.
16. E. Balagurusamy, 1995, "C^{++}" 1st ed, New Delhi, Tata Mc Graw Hill.
17. Merrit W Dean and Settle, 1986, " Instrumental methods of analysis", 6th ed., New York, CBS Publishers and distributors,
18. Mackie R.K. and Smith D.M., 1982 "Guide book to organic synthesis" London, ELBS,.

Paper II: PHYSICAL METHODS IN CHEMISTRY

Unit I

UV Visible spectroscopy - Instrumentation - Microstates - Term symbols and energy levels for d^1 - d^9 ions in cubic and square fields - intensity of bands - group theoretical approach to selection rules - effect of distortion and spin -orbit coupling on spectra - Evaluation of 10 Dq and β values for octahedral complexes of cobalt and nickel - applications to simple coordination compounds - applications to organic compounds and calculation of λ_{max} - charge transfer spectra.

IR and Raman spectroscopy - Instrumentation - preparation of samples and pellet making - applications of IR and Raman spectroscopy - combined uses of IR and Raman spectroscopy in structural elucidation of simple molecules like N_2O, ClF_3, NO_3^- ClO_4^- Predicting IR bands for simple organic molecules - effect of coordination on ligand vibrations - uses of group vibrations in the structural elucidation of metal complexes of urea, thiourea, cyanide, thiocyanate, nitrate, sulphate and dimethyl sulfoxide - effect of isotopic substitution on the vibrational spectra of metal carbonyls with reference to the nature of bonding, geometry and number of C-O stretching vibrations (group theoretical treatment) - Applications of Raman Spectroscopy. Photo electron spectroscopy - Principle - Auger electron spectroscopy - electron spectra in chemical analysis.

Unit II

NMR spectroscopy - Bloch equations, the quantum mechanical description of the NMR experiment, transition probabilities, Relaxation effects, Fourier transform NMR - measurements of T_1 and T_2. Effect of quadrupolar nuclei evaluation of thermodynamics and kinetic data using NMR techniques, second order spectra -Quantum mechanical treatment of coupling, effect of relative magnitudes of J on the spectrum of an AB and ABX molecules, double resonance experiment. Spectral simplification and determination of signs of coupling constants. Examples for different spin systems - chemical shifts and coupling constants (spin - spin coupling) involving different nuclei (^1H, ^{19}F, ^{31}P, ^{13}C) - elementary aspects of Solid State NMR.

NMR of paramagnetic molecules - isotropic shifts contact and pseudo contact interactions - lanthanide shift reagent. Characteristics of quadrupolar nucleus - effect of field gradient and magnetic field upon quadrupolar energy levels - NMR transitions applications - Basic principles and applications of NQR.

Sampling techniques, factors influencing group frequencies both internal and external quantitative studies, hydrogen bonding (intermolecular and intramolecular) conformational aspects in cyclic 1,2 -diols and 1,3 -diols, ^1H NMR spectroscopy - coupling constant - first order and second order splitting spin - spin splitting - dependence of J on dihedral angle - vicinal and geminal coupling constants - Karplus equation - long range, coupling constants, influence of stereo chemical factors on chemical shift of protons, simplification of complex spectra - double resonce techniques, shift reagents, chemical spin decoupling of rapidly exchangeable protons (OH, SH, COOH, NH, NH_2) - an elementary treatment of NOE phenomenon - 2D technique (COSY, NOESY and ROSY) ^{13}C NMR spectroscopy. Basic theory of FT - NMR - Relaxation - broad band decoupling. Off resonance decoupling and chemical shift correlations (CH, CH_2, CH_3, $=CH_2$, =C, aromatic). NQR - Basic Principles.

Unit III

EPR spectroscopy - Factors affecting the magnitudes of g and A tensors in metal species - Zero field spitting and Kramer's degeneracy - spectra of V(II) , Mn(II), Fe(II), Co(II), Ni(II) and Cu (II) complexes- applications of EPR to a few biological molecules containing Cu(II), Fe(II) and Fe(III) ions - spin densities and McConnel relationship - Applications of EPR to some simple systems such as CH_3, p-benzosemiquinone. Xe^{2+}

Moss Bauer spectroscopy - Isomer shifts - magnetic interactions - Mossbauer emission spectroscopy - application to iron and tin compounds.

Mass spectrometry - Instrumentation - resolution, EI and CI methods - base peak, isotopic peaks, metastable peak, parent peak, determination and use of molecular formula, recognition of molecular ion peak - FAB Fragmentation - general rules - pattern of fragmentation for various classes of compounds, McLafferty rearrangement, Importance of metastable peaks.

Unit IV

Diffraction Methods - Crystal symmetry - combination of symmetry elements - crystal classes - screw axis and glide planes - space group - crystal axes - crystal systems, unit cell, Bravais lattices, asymmetric unit - space group - Equivalent positions- relationship between molecular symmetry and crystallographic symmetry - basic concepts and examples.

X - Ray diffraction - The concept of reciprocal lattice and its applications - X-ray diffraction by single crystals - structure factor - determination of space group by symmetric phase problem in structure analysis - heavy atom method - Fourier synthesis - refinement of structure. Neutron diffraction - Magnetic scattering - applications and comparison with X-ray diffraction.

Electron diffraction - Basic principles and application to simple molecules - XeF_6, $Be(BH_4)_2$, ferrocene, Cr(II)acetate.

Unit V

Quantum Chemistry - The variation method and perturbation theory. Application to the helium atom; anti symmetry and exclusion principle, Slater determination, wave functions. Term symbols and spectroscopic states.

Born-Oppenheimer approximation Hydrogen molecular ion. LCAO - MO and VB treatments of the hydrogen molecule, electron density, forces and their role in chemical bonding, Hybridization and valence MO's of water, ammonia and methane. Huckel pi-electron theory and its applications to ethylene, butadiene and benzene, idea of self consistent fields.

Group theoretical representations and quantum mechanics. Vanishing of integrals. Spectroscopic selection rules for vibrational electronic, vibronic Raman spectroscopy, MO treatment of large molecules with symmetry.

Instrumentation and applications of Electro analytical techniques

Polarography, Amperometry, Cyclic voltammetry, Coulometry, Electrogravimetry, Potentiometry and Conductometry

Text Books

1. Huheey JE, Keiter EA and Keiter RA, 2000, Inorganic Chemistry, Principles of Structure and Reactivity, 4th edition, New Delhi, Pearson Education (Asia).
2. Silverstein RM and Webster FX, 2003, Spectrometric Identification of Organic Compounds, 6th edition, New York, John-Wiley and Sons Inc.
3. Kalsi PS, 1990, Stereochemistry Conformation and Mechanism, 4th edition, New Delhi, New Age International Publishers.
4. Straughan BP and Walker S, 1976, Spectroscopy vol: 1-3, London, Chapmann and Hall.
5. Drago RS, 1980, Physical Methods in Chemistry, New Delhi, W. B. Saunders.

Reference Books

1. Rifi MR and Covitz FH, 1974, Introduction to Organic Electrochemistry, New York, Marcel Dekker.
2. Kemp W, 1993, Organic Spectroscopy, 3rd edition, London, ELBS with Macmillan.
3. Cotton FA, Wilkinson G, Murillo CA and Bochman M, 2003, Advance Inorganic Chemistry, 6th edition, New York, John-Wiley and Sons Inc.
4. Kalsi PS, 1999, Stereochemistry and Mechanism Through Solved Problems, 3rd edition, New Delhi, New Age International Publishers.
5. Sutton D, 2000, Electronic Spectra of Transition Metal Complexes, New Delhi, Narosa Publishing House.
6. Nasipuri D, 2000, Stereochemistry of Organic Compounds, New Delhi, Narosa Publishing House.
7. Bancroft M, 1973, Mossbauer Spectroscopy, New Delhi, Tata McGraw-Hill Publishing Company.
8. Wheatly PJ, 1959, The Determination of Molecular Structure, London, Oxford at the Clarendon Press.
9. Ebsworth EAV, 1987, Structural Methods in Inorganic Chemistry, 3rd ed, London, ELBS.

Paper III: RECENT TRENDS IN CHEMISTRY

Unit I: NANO CHEMISTRY

Introduction - types of nanotechnology and nano machines - molecular nanotechnology - scanning electron microscope(SEM) - modern transmission electron microscope(TEM) - scanning probe microscope(SPM) - atomic force microscope (AFM) - nano dots - nano materials - preparation - plasma arching - sol gels - electro deposition - ball milling - applications of nano materials - carbon nano tubes - molecular switches - rotaxanes and catenanes - lithography - nano bio metrics - future applications.

Unit II: MACROCYCLICS

Introduction - definition - design and synthesis of macro cyclic ligands (1+1 and 2+2) - synthetic procedures - direct macro cyclic synthesis - synthesis by coordination template effect - thermodynamic and kinetic effects - transamination - transmetalation - anion template effect - template potential of transition and inner transition metals - macro cyclic systems - macro cycles types - crown ethers - cryptands - catenands - cage macro cycles - bi nucleating macro cycles - compartmental ligands- natural macro cyclic systems - Host - Guest chemistry - sequestration - molecular mechanics and molecular graphics - technique in the design of macro cycles .

Unit III: SONOCHEMISTRY AND MICROWAVE INDUCED SYNTHESIS

Sono chemistry - introduction - instrumentation - types of sono chemical reactions in homogeneous and heterogeneous systems - synthetic application; esterification, saponification, hydrolysis substitution, addition allylation, oxidation, reduction, coupling reaction, Cannizaro reaction, Strecker synthesis - Reformatsky-Barbier reaction - Sonoluminescence, Sonocatalyst, application in nanochemistry.

Microwave synthesis - introduction - instrumentation - microwave assisted reactions in water: Hoffmann elimination, hydrolysis, oxidation of toluene and alcohols and saponification. Microwave assisted reactions in organic solvents: Esterification, Fries rearrangement, Claisen rearrangement, Diels Alder reaction, decarboxylation. Solvent free microwave reactions: deacylation, deprotanation, saponification of esters, synthesis of nitriles from aldehydes, synthesis of anhydrides from dicarboxylic acids, reduction, synthesis of hetero cyclics.

Unit IV: CHEMINFORMATICS

Basics of Cheminformatics: introduction - evolution - history of chemical information science - uses of cheminformatics.

Drug design and discovery: development of a drug - pharmacodynamics - biological testing and bioassays - chemical parameters in drug design - physico chemical parameters in drug design - structure based drug design - drug discovery

Unit V: ELECTRO ORGANIC CHEMISTRY

Merits and demerits of electro chemical reactions: Electrolysis, electro deposition, constant current electrolysis, controlled potential electrolysis, cell designing - types of electrodes and their characterisation - Pt, Ni, Graphite, glassy carbon, lead dioxide, titanium dioxide, ruthenium oxide and coated polymer electrodes, Supporting electrolytes and their characterisation, Solvents role in electro chemical reactions, Electrochemical E and C processes.

Cathodic reduction of carbonyl compounds and nitro compounds. Factors influencing cathodic reduction. Anodic oxidation of organic compounds - anodic aromatic side chain oxidation of toluene - Aromatic ring oxidation - alkoxylation - acetoxylation - halogenation - acetoamylation - oxidation of aliphatic - Factors influencing anodic oxidation, indirect electrooxidation using Mn, Cr, Fe, Cerium salts, bromonium and iodinium salts.

REFERENCES

Unit I

1. Nanotechnology - Basic Science and Emerging Technologies, MichWilson, Kamali Kannangari, Geoff Smith, 2005, overseas press India private ltd.

Unit II

2. Lindloy, L.F.,1989, The chemistry of macro cyclic ligand complexes, Cambridge university press, N.Y.
3. Alexander V, Chemical reviews, 1995, 95, (2), 273-676.

Unit III

4. V. K. Ahluwalia and M. Kidwai, New Trends in Green Chemistry, II edition, Anamaya publishers, New Delhi, 2006
5. V. K. Ahluwalia and Renu Aggarwal, Organic Synthesis - Special Techniques, II edition, Narosh publishing house, New Delhi, 2006

Unit IV

6. Nourse. J. G, et.al. J. Chem. Inf. Comput. Sci., 32 (1988)
7. Siani, M. A, et.al. J. Chem. Inf. Comput. Sci.,Vol.34 (1994)
8. Study Material - Institute of Chem informatics Studies

Unit V

9. T. Shono, Electro Organic Chemistry as a new tool in Organic Synthesis, Vol 20, Springer- Verlag, NY, 1984
10. Norman L. Weinberg, Technique of electro organic synthesis, Part - 1 & Part - 2, John. Wiley & sons.

Paper-IV: THERMODYNAMIC AND PHYSICAL PROPERTIES OF LIQUID SOLUTIONS

Dr X. Rosario Rajkumar

Unit I: Ultrasonic velocity studies in liquids and liquid mixtures

Ultrasonic Interferometer - Principle and measurement of ultrasonic velocity in liquids and liquid mixtures. Ultrasonic velocity and hydrogen bonding in solutions. Ideal and non-ideal solutions - laws - Raoult's law, Henry's law. Calculation of excess volume, Internal pressure, free volume, free length, and deviation in isentropic compressibility

Unit II : Theories of liquid state

Cell theory - Hole theory - Lattice model - Prigogine's model - Flory's theory- Recent Theories from Literature.

Unit III : Basic concepts in solution chemistry

Concentration units - molarity, molality, mole fraction, volume fraction, percentage by weight, percentage by volume - Van der Waals forces,dipole-dipole interaction, dipole induced dipole interaction, London dispersion forces, hydrogen bonding - Measurement of density, viscosity and heat of solution by calorimetry

A review of liquid mixtures with reference to excess volume and heat of mixing

Unit IV: Solutions of Electrolytes

Chemical Potential - Activity coefficients - Debye Huckel Theory - Debye Huckel Limiting Law - Thermodynamic functions from Debye Huckel theory (D-H) - Critical Examination of D-H theory - Modification in D-H theory Solutions of Electrolytes.

Unity V: Review on Excess Properties of Solutions

Review on excess properties in Chemical Reviews Ch.1 (1971) -Battino, R. - Measurement of vapour pressure of liquids using isoteniscope.

Text Books

1. Gupta MC, 1990, "Statistical Thermodynamics", Madras, Wiley Eastern Ltd.
2. Glasstone S, 2002, "Thermodynamics for Chemists", New Delhi, Affiliated East-West press pvt,Ltd.

References

1. Rowlinson JS, 1971, "Liquids and liquid mixtures", London, Butterworth.
2. Findlay A, Practical Physical chemistry.
3. Srivastava KC, 2001, "Hand book of Ultrasonic testing", 1st edition International Inspection services, .
4. Kinsler LE and Frey AR, 1991, "Fundamentals of Acoustics", 2nd edition, Madras, Wiley Eastern Ltd.

Paper-IV: REACTIVITY OF ETHER LINKAGE

Dr S Raja

Unit I

Electro negativity order of elements - acid, base concepts - Lewis concept of acids and bases - reaction intermediates - formation and stability of carbocation and carbonium - reactions of carbocations by abstracting hydride - electronic and steric effect - concept of oxidation - reduction electronic concept -effect of polarity of solvents on type of reactions - purification of organic solvent like benzene, nitro benzene and acetonitile

Unit II

Aromatic electrophilic substitution reaction - formation of π-complexes and σ complexes - electrophilic substituion in different homo-aromatic and Hetero aromatic compounds - aliphatic electrophilic substitution reactions - S_Ni mechanism - mechanism of elimination reaction E_1, E_2 and E_1CB.

Unit III

IR, NMR spectroscopy in structural determination of organic compounds - Principles of TLC, thin layer chromatography and column chromatography and techniques for separating the different components present in the organic mixture - Principle of using different solvents of varying polarity.

Unit IV

Different methods of formation of acetal - mechanism of acetal formation - stability of acetals - oxidation of ether by $KMnO_4$, $KBrO_3$ alkalies - metal halides.

Unit V

Mechanism of action of N_2O_5 on methyl phenethyl ether - mechanism of reaction of hypochlorous acid on anisole - migration of halogen in ortho rearrangement - action of $SnCl_4$ on acetals - Hunsdiecher reaction - mechanism evidence and limitations of Hunsdiecher reaction.

Text Books

1. March J, 1992, *Advanced Organic Chemistry* (4th ed), New York, John Wiely & Sons.
2. Kemp W, 1993, Organic Spectroscopy, 3rd edition, London, ELBS with Macmillan.

Refereces

1. Gould.E.S, 1959, *Mechanism and Structure in Organic Chemistry,* New York, Holt Rinehart and Winston.
2. Pine S.H.et,al, 1986, *Organic Chemistry* (Fourth Edition), Singapore, McGraw-Hill Book Company.
3. Dyer JR, 1984, *Applications of Absorption Spectroscopy of organic compounds*, New Delhi, Prentice Hall of India.

Paper-IV: KINETICS AND MECHANISM

Dr. N. Mathiyalagan

Unit I

Empirical treatment of reaction rates: effect of concentration- rate expression-product study-stoichiometry.

Experimental methods of measuring reaction rates: Instrumental method of analysis-chemical methods-determination of order. Relation between rate and mechanism.

Unit II

Activated complex theory- current status-extension- applications. Entropy of activation-enthalpy of activation.

Reactions in solutions: factors determining reaction rates in solution. Reaction between ions, dipoles-effect of ionic strength--primary and secondary salt effect-kinetic isotope effect-primary and secondary isotope effect.

Unit III

Complex reactions: steady state treatment- microscopic reversibility-detection and estimation of radicals in reaction system. Homogeneous catalysis in solution: Mechanism of acid-base catalysis-catalytic constant-general and specific and base catalysis. Bronsted catalysis law-acidity function.

Unit IV

Hammett and Taft equation: Influence of substituents on reaction rates-electronic theory of organic reactivity-influence of substituents on the energy of activation-LFER substituent constant-reaction constant for aromatic and aliphatic systems. Applications of Hammett and Taft equations in reaction mechanism. Linear free energy relations and Bronsted catalysis law. Iso kinetic relationship: Effect of temperature on reaction rates-reaction series-enthalpy and entropy relationship. Exner plot-isokinetic temperature.

Unit V

Some reaction mechanism in solution: Hydrolysis of esters and acetals, oxidation of alcohols and aldehydes by N- halogeno compounds like NBS, NCS, CBT etc.

Text books

1. Laidler KJ, 1984, Chemical Kinetics, 3rd edition, New Delhi, Tata McGraw-Hill Publishing Company.
2. Frost A and Pearson RG, 1970, Kinetics and Mechanism, John-Wiley Eastern.

References

1. Indian J. Chem., 1986. 25, pp 478.
2. Can. J. Chem., 1969. 47, pp 694.
3. Indian J. Chem. 1976. 14B, pp 898.

Paper-IV: ADVANCED COORDINATION CHEMISTRY

Dr S R Bheeter

Unit I

Methods of preparation of coordination compounds - Analysis and determination of molecular formula - Volumetric, gravimetric and colourimetric methods - Conductance and magnetic measurements of complexes

Unit II

Theories of coordination - CF, MO, LF Theories - Merits and demerits - σ donor and π acceptor ligands - Carbonyls - Nitrosyls - Cyanides - Triphenyl phosphine complexes - Organo metallic compounds - Allene, alkyne and allyl ccomplexes

Unit III

Special application to the study of coordination compounds - Electronic spectra - IR spectra - NMR spectra - ESR spectra - Moss baur spectra - PES

Unit IV

Kinetics and reaction mechanism in coordination compounds - S_N1, S_N2, S_NCB mechanisms - Trans effect - Electron transfer and electron exchange reactions - Catalysis by organometallic compounds

Unit V

Transition metal ion in biology - Iron enzymes - structure and their functions - Model system for molecular activation and corresponding biochemical system.

Text Books

1. Kettle SFA, Physical Inorganic Chemistry: A Coordination chemistry Approach, 1996, Oxford, Specktrum.
2. Drago R.S., 1977, Physical methods in inorganic chemistry, London, Saunders Golden Sunburst Series, W.B.Saunders Company.
3. Lewis J and Wilkinson RG (Editiors), 1960, Modern coordination chemistry, Principles and Methods, New York, Interscience Publishers, Inc.

References

1. Lee JD, 1988, *Concise inorganic chemistry,* (sixth edition) London, ELBS.
2. Huheey JE., 1972, *Inorganic chemistry Principle structure and reactivity*, (second edition), New York, Harper & Row publishers.
3. Cotton F.A. and Wilkinson G., 1988, *Advanced inorganic chemistry,* (Third Edition) London, John Wiley & sons.

Paper-IV: REACTIVITY OF ETHER LINKAGE

Dr K Joseph Santhanaraj

Unit I

Electro negativity order of elements - acid, base concepts - Lewis concept of acids and bases - reaction intermediates - formation and stability of carbocation and carbonium - reactions of carbocations by abstracting hydride - electronic and steric effect - concept of oxidation - reduction electronic concept -effect of polarity of solvents on type of ractions - purification of organic solvent like benzene, nitro benzene and acetonitile

Unit II

Aromatic electrophilic substitution reaction - formation of π-complexes and σ complexes - electrophilic substituion in different homo-aromatic and Hetero aromatic compounds - aliphatic electrophilic substitution reactions - S_Ni mechanism - mechanism of elimination reaction E_1, E_2 and E_1CB.

Unit III

IR, NMR spectroscopy in structural dermination of organic compounds - Principles of TLC, thin layer chromatography and column chromatography and techniques for separating the different components present in the organic mixture - Principle of using different solvents of varying polarity.

Unit IV

Different methods of formation of acetal - mechanism of acetal formation - stability of acetals - oxidation of ether by $KMnO_4$, $KBrO_3$ alkalies - metal halides.

Unit V

Mechanism of action of N_2O_5 on methyl phenethyl ether - mechanism of reaction of hypochlorous acid on anisole - migration o halogen in orton rearrangement - action of $SnCl_4$ on acetals - Hunsdiecher reaction - mechanism evidence and limitations of Hunsdiecher reaction.

Text Books

1. March J, 1992, *Advanced Organic Chemistry* (Fourth Edition), New York, John Wiely &sons.
2. Kemp W, 1993, Organic Spectroscopy, 3rd edition, London, ELBS with Macmillan.

Refereces

1. Gould, E.S, 1959, *Mechanism and Structure in Organic Chemistry,* New York, Holt Rinehart and Winston.
2. Pine S.H.et,al, 1986, *Organic Chemistry* (Fourth Edition), Singapore, McGraw-Hill Book Company.
3. Dyer JR, 1984, *Applications of Absorption Spectroscopy of organic compounds*, New Delhi, Prentice Hall of India.

Paper-IV: ADVANCED STUDIES OF MACROCYCLIC COMPLEXES

Dr M Amaladasan

Unit I

Methods of preparation of coordination compounds - Analysis and determination of molecular formula - Volumetric, gravimetric and colourimetric methods - Conductance and magnetic measurements of complexes

Unit II

Theories of coordination - CF, MO, LF Theories - Merits and demerits - Macrocycles and their classifications - Synthesis of Macrocycles - Properties and applications

Unit III

Special application to the study of coordination compounds - Electronic spectra - IR spectra - MR spectra - ESR spectra - Mossbaur spectra - PES

Unit IV

Kinetics and reaction mechanism in coordination compounds - S_N1, S_N2, S_NCB mechanisms - Trans effect - Electron transfer and electron exchange reactions - Catalysis by organometallic compounds

Unit V

Transition metal ions in biology - Iron enzymes - structure and their functions - Model system for molecular activation and corresponding biochemical system.

Text Books

1. Lee JD, 1998, *Concise inorganic chemistry,* (sixth edition), London, ELBS.
2. Huheey JE., 1972, *Inorganic chemistry Principle structure and reactivity*, (second edition), New York, Harper & Row publishers.
3. Drago RS., 1977, *Physical methods in inorganic chemistry*, London, Saunders Golden Sunburst Series, W.B.Saunders Company.

References

1. Cotton FA and Wilkinson G., 1988, *Advanced inorganic chemistry,* (Third Edition), London, John Wiley & sons.

Paper-IV: ORGANIC REACTION MECHANISM

Dr N Xavier

Unit I: Basic concepts in organic chemistry

Hard and Soft Acid Base principles - Types of organic reactions - substitution, elimination and addition reactions - Reactive intermediates - stereochemical and conformational effects on reactivity and specificity; reaction with diboranes and peracids - Michael reaction- Robinson annulation - Reacativity umpolung - acyl anion equivalent- Molecular rearrangements involving electron difficient atoms.

Unit II: Reagents and reactions

Functional group transformations - Reagents for the inter conversion of various groups - Special and specific oxidizing agents, reducing agents and organo metallic compounds for the inter conversions - The survey of reactions and reagents - Gilman's reagent - LDA - DCC - 1,3-dithiane - Trimethyl silyl iodide - Wilkinson's catalyst - OsO_4 - DDQ - SeO_2.

Unit III: Aromatic character and Aromatic substitution reactions

Concepts of aromaticity - Reactions of aromatic compounds - Aromatic electrophilic and nucleophilic substitution reactions - Substituent effects on aromatic substitution reactions

Unit IV: Reactivity of phenol

Reactions of phenol - substitution reactions of phenol - Special emphasize on Reimer Tiemann reactions - Kolbe reaction - Acylation - Chloro methylation sigmatropic shift - Reactions resembling Reimer Tiemann reaction - Detailed mechanism of the reaction.

Unit V: Survey of Reimer Tiemann reaction

Special feature of Reimer Tiemann reaction - Factors influencing the reaction - Possible conditions to enhance the yield of the products - Industrial viability of the reaction conditions - Commercial importance of the reaction products.

Text Books

1. March J, 1992, *Advanced Organic Chemistry*, Fourth edition, New York, John Wiley and sons.
2. Gould ES, 1959, *Mechanism and Structure in Organic Chemistry,* Now York, Holt Rinehart and Winston.

References

1. Pine SH etal., 1986, *Organic Chemistry*, Fourth edition, Singapore, McGraw Hill Book Company.

Paper-IV: PHYSICAL METHODS IN INORGANIC CHEMISTRY

Dr A Paul Raj

Unit I

Methods of preparation of coordination compounds - Analysis and determination of molecular formula - Volumetric, gravimetric and colourimetric methods - Conductance and magnetic measurements of complexes

Unit II

Theories of coordination - CF, MO, LF Theories - Merits and demerits - σ donor and π acceptor ligands - Carbonyls - Nitrosyls - Cyanides - Triphenyl phosphine complexes - Organo metallic compounds - Allene, alkyne and allyl complexes

Unit III

Special application to the study of coordination compounds - Electronic spectra - IR spectra - NMR spectra - ESR spectra - Moss baur spectra - PES

Unit IV

Kinetics and reaction mechanism in coordination compounds - S_N1, S_N2, S_NCB mechanisms - Trans effect - Electron transfer and electron exchange reactions - Catalysis by organometallic compounds

Unit V

Transition metal ion in biology - Iron enzymes - structure and their functions - Model system for molecular activation and corresponding biochemical system.

Text Book

1. Drago R.S., 1977, *Physical methods in inorganic chemistry*, London, Saunders Golden Sunburst Series, W.B.Saunders Company.

References

1. Lee JD, 1988, *Concise inorganic chemistry,* (sixth edition) London, ELBS.
2. Huheey JE., 1972, *Inorganic chemistry Principle structure and reactivity*, (second edition), New York, Harper & Row publishers.
3. Cotton F.A. and Wilkinson G., 1988, *Advanced inorganic chemistry,* (Third Edition) London, John Wiley & sons.

Paper-IV: CORROSION INHIBITION ON METALS

Dr A Peter Pascal Regis

Unit I

Corrosion - definition- costs of corrosion - economic losses - Human life and safety - Types of corrosion: dry corrosion - wet corrosion - mechanisms - galvanic corrosion, concentration cell corrosion, atmospheric corrosion, soil corrosion, pitting corrosion, inter granular corrosion, waterline corrosion, stress corrosion, microbial corrosion

Unit II

Factors influencing corrosion: Nature of metals: Position in galvanic series - over voltage - relative areas of anodic and cathodic parts - purity of metals - physical state of metal - nature of surface film - solubility of corrosion products.

Nature of corroding environment temperature - Humidity - presence of impurities in atmosphere - influence of pH - nature of ions present conduction of the corroding medium - formation of oxygen concentration cell.

Unit III

Corrosion control: Proper designing - use of pure metals - using metal alloys - cathodic protection -sacrificial anodic protection method - impressed current cathodic protection

Use of inhibitors: inhibitors - definition - classification - due to Putilova - due to Deano - anodic - cathodic - mixed

Unit IV

Theories of inhibition of corrosion: Adsorption theory and molecular structure - hydrogen over potential theory, film formation theory - synergistic effect - example - corrosion inhibition in neutral gaseous environments - chromate, molybdates, nitrite, phosphate, silicate, cations, organic inhibitors carboxylate and tannins.

Unit V

Phospates as inhibitors: Phosphonates: definition - reasons for using Phosphonates as inhibitors - Use of HEDP, ATMP, ethyl phosphonic acid, 2-carboxyethyl phosphonic acid as corrosion inhibitors.

Text Books

1. Antropov.L., 1972, *Theoretical electro chemistry*, Moscow, Mir Publishers.

References

1. Bockris.J.O.M. and Reddy A.K.N, 1970, *Modern Electro chemistry* Volume I and II, New York, Plenum Press.

Paper-IV: NATURAL PRODUCTS CHEMISTRY

Dr V Alex Ramani

Unit I: Plants and Plant Products

Classification of Plants - Nomenclature - Cells - Tissues - Structures and Functions of Cells and tissues - Primary Metabolites - Secondary Metabolites - Microorganism- Types - Microbes and Man - Biological Activities - Microbial Studies - Techniques - Interpretation of Results

Unit II: Methods of Plant Analysis I

Methods of Extraction - Cold Percolation Method - Soxhlet Method - Methods of Isolation - Methods of Separation

Chromatography - Paper Chromatography - Column Chromatography - Thin layer Chromatography - Gas Chromatography - High performance Liquid Chromatography

Electro phoresis - Paper and Gel Electrophoresis - Distillations - Steam Distillation - Fractional Distillation - Vacuum Distillation - Crystallization Techniques

Unit III: Methods of Plant Analysis II

UV-VIS spectroscopy - IR Spectroscopy - Proton and Carbon-13 NMR Spectroscopy - Mass Spectroscopy - X-ray and Neutron Diffraction studies - Optical studies - Qualitative and Quantitative Analyses - Interpretation of Results

Unit IV: Phenolic Compounds and Terpenoids

Methods of separation, isolation and identification - Phenolics - Phenyl propanoids - Anthocyanins - Flavonoids - Xanthones - Stilbenes - Chemical conversions of these compounds - Structure Elucidation of Quercetin, Vitexin and Naringin

Methods of separation, isolation and identification - Monoterpenes - Sesquiterpenes - Diterpenes - Triterpenoids - Steroids - Carotenoids - Chemical convesions of these compounds - Structure Elucidation of Menthol and Carotol.

Unit V: Nitogen Compounds, Sugars, Lipids and other related Compounds

Methods of separation, isolation and identification - Amino acids - Proteins - Peptides - Amines - Alkaloids - Cyanogenic glycosides - Purines - Pyrimidines - Cytokinins - Chlorophylls - Chemical conversions of these comnpounds - Structure Elucidation of Nicotine and Cytisin.

Methods of separation, isolation and identification - Monosaccharide - Disaccharide - Polysaccharides - Shikimic acids - Quinic acid - Fatty acids - Polyacetylenes - Sulfur compounds - Chemical conversions of these compounds - Structure Elucidation of Shikimic acid and Rhanmonse.

Text Books

1. Peach K and Tracey MV (eds.), 1956-1964, *Moderne der pfranzenanalyse*, Berlin, Spinger verlag.
2. Krishnasamy N.R, 1999, *Chemistry or Natural Products,* Hyderabad, University Press.
3. Boyer RF, 1993, *Modern Experimental Biochemistry,* II Ed., California, The Benjamin /Cummings publishing company Inc.
4. Furniss BS, Hannaford AJ, Smith PWG and Tatchell AR, 1989, Vogel's *Text book of Practical Organic Chemistry*, V Ed., Essex, England, ELBS with Longman.
5. Harborne JB, 1988, Phytochemical Methods: *A Guide to Modern Techniques of Plant Analysis,* II Ed., London and New York, Chapman and Hall.

References

1. Finar I.L. *Organic Chemistry*, Vol. 2. ELBS London.
2. Raphael Ikan, 1969, *Natural Products: A Laboratory Guide*, Jerusalem, Israel University Press.
3. Jeffrey C, 1982, *An Introduction Plant Taxonomy*, II Ed., Cambridge, Cambridge University Press.
4. William J and Sham M, *1976, Microorganisms*, London, Mills and Boon Limited.
5. Ari Koskinen, 1993, *Asymmetric Synthesis of Natural Products,* Chichester, New York, Brisbane, Toronto, Singapore, John Wiley and Sons.

Paper-IV: ADVANCED COORDINATION CHEMISTRY

Mr A N Paul Angelo

Unit I: Synthesis of Novel Coordination Compound

Design ad Synthesis of macrocyclic Ligands - Synthetic Procedures - Direct Macrocyclic synthesis, Microwave assisted synthesis - Metal ion template synthesis - Macrocyclic systems

Macrocycles with pendant functional group - Catenands, Cage macrocycles, Cryptands and Crown Polyethers - Binucleating macrocycles - Compartmental Ligands. Natural macrocycles - Host-guest chemistry- macrocyclic host and non-metallic guests.

Unit-II Theories of Coordination Compounds and Mechanisms

Crystal Field , Ligand Field, Molecular Orbital Theories and Angular Overlap - Model Mechanism of Electron Transfer Reactions - Innersphere and Outer sphere electron - transfer mechanisms - Substitution reaction in square planar complexes, trans effect - Oxidative addition and insertion reactions.

Unit-III Determination of Electronic Structure and Geometry of Coordination Compounds-I

Electronic spectroscopy: Electronic states and spectra of Td and Oh complexes, charge transfer spectra LMCT, MLCT, crystal field spectra. Evaluation of values in Co(III) Oh and Ni(II) Oh complexes Dq xy and Dq z in tetragonally distorted cobalt(II) octahedral complexes. Infrared and Raman spectroscopy: Structural diagnosis: IR spectral assignment of coordinated ligands in metal complexes and differentiation of isomers (CN/NC, OCN/NCO, SCN/NCS, CNO/ONC, NO_2/ONO

NMR Spectroscopy - Application of spin-spin coupling to structure determination. NMR of paramagnetic transition metal ion complexes , scalar shift and covalency. Lanthanide shift reagents. ESR anisotropy in the g-value, hyperfine and zerofield effect on the spectrum, Survey of the EPR spectrum of first row transition metals.

Unit-IV Determination of Electronic Structure and Geometry of Coordination Compounds-II

Magnetic Behaviour of Coordination Compounds. Methods of determining magnetic susceptibility, and electron states - Electrochemical methods of studying coordination compounds. Electrochemical and electrochemical reversibility. Pulse polarography, AC Polarography, Cyclic voltammetry. Electrochemical synthesis of complexes. Coupled chemical reactions - EC, CE and ECE mechanisms. Photoelectron spectroscopy and X-PES - Study of chiral coordination compounds by ORD and CD - Mass Spectroscopy - CIMS, EIMS and FAB-MS.

Unit-V: Catalysis of Organometallic compounds and Bio-inorganics

Ziegler - Natta polymerization, cyclooligomerization , olefin isomerization, metathesis and polymer bound catalysis. The oxygen carriers- hemoglobin and myoglobin and synthetic oxygen carriers. Electron transfer agents - Cytochromes, iron-sulphur proteins. Mechanism

of electron transfer reactions. Nitrogen Fixation. Essential and trace elements in biological systems. Chelate therapy. Applications.

References

1. Lindoy.L.F, 1989, The Chemistry of Macrocyclic Ligand Complexes, Cambridge University Press, N.Y.
2. Huheey J.E., 1988, Inorganic Chemistry, 4th Edition . Harper and Row, NY
3. Cotton.F.A and Wilkinson, G 2001Advanced Inorganic Chemistry, 6th Ed., Wilrey Interscience, NY,
4. Purcell.K.F and Kotz. J.C. 1976, Inorganic Chemistry, Saunders.
5. Lever.A.B.P, 1984, Inorganic Electronic Spctroscopy, 2nd Ed., Elsevier Publishing Company, Amsterdam
6. Nakamoto. K, 1986, Infrared and Raman Spectra of Inorganic and Coordination Compounds, 4th Ed., Eiley Interscience
7. Basolo F and Pearson .R.G, 1967, Mechanism of Inorganic reactions, 2nd Ed., Wiley Eastern. New Delhi.
8. Kissinger.P.T, and Heineman.W.B, 1984, Laboratory Techniques in Electroanalytical Chemistry, Editors, Marcel Dekker, Inc., New York
9. Drago R.S., 1977, Physical Methods in Chemistry, Saunders, Amsterdam.
10. J. Chem. Educn., 1983, 60, 252-308.
11. J. Chem. Educn., 1983, 60, 687-706.
12. Eichhorn G.L., Ed., 1976, Inorganic Biochemistry, Elsevier, Amsterdam.

Paper-IV: THERMODYNAMICS OF LIQUID SOLUTIONS

Mr A Rose Venis

Unit I: Chemistry Of Solutions

Concentration units- molarity, molality, mole fraction, volume fraction, percentage by weight and volume. Ideal and non-ideal solutions-Raoult's law, Henry's law, models in ideal and non-ideal solutions, their miscibility's, thermal properties, Binary and ternary liquid mixtures.

Unit II: Theories of Liquid Mixtures

Cell theory, Hole theory, lattice model, Prigogine's model, Flory theory, scaled particle theory, free length theory, Kharare equation, Kalidoss-Jacobson theory. Types of interactions in solutions.

Unit III: Review on Thermodynamic Properties

Review of thermodynamic properties of solutions. Liquid solutions of non-electrolytes and electrolytes- activity coefficient- Deby- Huckel theory and its implications- thermodynamics of mixing. Measurement of density, viscosity, heat of solution, heat of mixing and vapour pressure.

Unit IV: Ultrosonic Studies in Liquid Mixtures

Ultrasonic interferometer- principle, instrumentation, generation of ultrasonic waves, measurement of velocity, ultrasonic transducers. Calculation of excess volume, internal pressure, isentropic compressibility and its deviation, free volume, free length, relative association, acoustic impedance, molar sound so\peed, isothermal compressibility, thermal expansion coefficient, partial and apparent molar volume, excess viscosity, excess molar Gibbs free energy of activation, stability constants of complexes. Relation of ultrasonic velocity with hydrogen bonding, phases, boiling points, molecular interactions and electrolytes.

Unit V Applications of Ultrasonic Sound Waves

Ultrasonic testingn - Laser ultrasonic- ultrasonics in medicine, biology and industry. Sonochemistry.

Text Books

1. Gupta MC, 1990, Statistical Thermodynamics, Madras, Wiley Eastern Ltd.
2. Glasstone S, 2002, Thermodynamics for Chemists, New Delhi, East-West Press Ltd.
3. Sindhu Sadu, Ultrasonic velocity studies in liquids and their correlation with structural aspects, New Delhi, Publishing House.

References

1. Rowlinson JS, 1971, Liquids and liquid mixtures, London, Butterworth.
2. Findlay A, Practical Physical chemistry.
3. Srivastava KC, 2001, Hand book of Ultrasonic testing, International Inspection services, 1st ed.
4. Kinsler LE and Frey AR, 1991, Fundamentals of Acoustics, 2nd ed, Wiley Eastern Ltd.

Paper-IV: PHYSICAL METHODS IN INORGANIC CHEMISTRY

Prof. S. Denis Arockiaraj

Unit I

Methods of preparation of complexes-physical methods of determination of molecular formula-conductance, magnetic measurements.

Unit II

Theories of coordination compounds-VBT, CFT, MOT, LFT-merits and demerits. Sigma donor and pi-acceptor ligands-carbonyls, nitrosyls, cycanides, triphenylphosphine complexes

Unit III

Applications of NMR, IR, Mossbauer, PES, ESR spectroscopic methods in the study of coordination complexes

Unit IV

Kinetics and reaction mechanism in coordination complexes-S_N1, S_N2, S_N1_{CB}. Theories and applications of trans effect-inner sphere and outer sphere electron transfer reactions-two electron transfer reactions-catalysis by organometallic compounds

Unit V

Bioinorganic chemistry-structure and functions of chlorophyll, haemoglobin, myoglobin, cyctochromes and iron enzymes

References

1. Drago R S. 1977, Physical Methods in Inorganic Chemistry, London, Saunders Golden Sunburst Series, W.B Saunders Company
2. Lee J D. 1988, Concise Inorganic Chemistry (Sixth Edition), London, ELBS.
3. Huheey J E. 1972 Inorganic Chemistry Principles of Structure and Reactivity (Second Edition), New York, Harper and Row Publishers.
4. Cotton F A and Wilkinson G. 1988, Advanced Inorganic Chemistry (Third Edition), London, John-Wiley & Sons.

Paper-IV: ELECTRO ORGANIC CHEMISTRY

Prof. S. Antony Sakthi

Unit I: Basic concepts of electroorganic chemistry

The contents of an electrolytic cell, electrode materials, anodes, cathodes. Electrolytic media-aqueous and non-aqueous media, Reference electrodes, salt bridges, Liquid-Junction potentials. Application of reference electrodes, diaphragms, permeable membranes and semi-permeable membranes. Designing of simple special cells.

Unit II: Electrochemical oxidation of some organic compounds

Oxidation of phenols, alcohols and glycols. Kolbe reaction, oxidation of carbonyl compounds - aldehydes, ketones, esters and lactones.

Unit III: Electrochemical reduction of some organic compounds

Carbon-Carbon bond formation reactions- acid and base catalyzed condensations. Carbon-heteroatom bond formation reactions-Pericyclic reactions

Unit IV: Aomatic substitution reactions

Concepts of aromaticity, electrophilic substitution of aromatic compounds (like chlorination, bromination and sulphonation). Substituent effects on aromatic electrophilic substitution.

Unit V: Separation and characterization techniques

Chromatographic techniques. TLC, column chromatography, paper chromatography, high performance liquid chromatography (HPLC)-principle, methods and applications of ^{1}H NMR, ^{13}C NMR, FT-IR and UV spectra.

References

1. Norman L. Weinberg, Techniques of electroorganic synthesis. Part I and Part II, 1975, John Wiley and Sons.
2. Mollwo Perkin F, Practical methods of electro organic chemistry, 1905, Longmans, Green and Co.
3. March J. 1992, Advance Organic Chemistry (Fourth Edition), New York, John-Wiley & Sons.

Paper-IV: ORGANIC SYNTHESIS

Dr. A. Edwin Vasu

Unit I

Basic concepts of organic synthesis-reactants, reagents (nucleophiles and electrophiles)-types of reactions-substitutions, eliminations, rearrangements and additions- Effects of substrate structure, attacking agents, solvent nature and other variables on the course, mechanism and rates of reactions

Unit II

Survey of functional group interconversions in organic chemistry-Protection and deprotection of functional groups in organic synthesis

Unit III

Carbon-Carbon bond formation reactions- acid and base catalyzed condensations. Carbon-heteroatom bond formation reactions-Pericyclic reactions

Unit IV

Reterosynthetic analysis-synthons-donor and acceptor synthons-disconnection approach. Reterosynthetic analysis of acyclic and cyclic compounds-one group and two group disconnections- Selective and controlled oxidation and reduction of various functional groups.

Unit V

Spectrometric methods for determining the structure of organic compounds-IR, NMR, Mass and UV. Methods of purification, separation-principles of TLC and column chromatographic techniques-Microwave assisted organic synthesis

References

1. March J. 1992, Advance Organic Chemistry (Fourth Edition), New York, John-Wiley & Sons.
2. Gould E S. 1959, Mechanism and Structure in Organic Chemistry, New York, Holt-Reinhart and Winston
3. Warren S. 1988, Organic Synthesis: The disconnection Approach. New York, John-Wiley.
4. Silverstein and Bassler, 2004, New York, Spectrometric Identification of Organic Compounds (sixth edition), John-Wiley & Sons.
5. Smith M B. 1994, Organic Synthesis, New York, McGraw-Hill International.

Paper-IV: ORGANIC REACTION MECHANISM

Mr. M. Jerald Antony Joseph

Unit - I: Basic concepts in organic chemistry

Acid Base concept - Hard and Soft Acid Base principle - Types of organic reaction - substitution, elimination and addition reactions - Reactive intermediates - stereochemical and conformational effects on reactivity and specificity - Reactions with peracids - Molecular rearrangements involving electron deficient atoms

Unit - II: Reagents and reactions

Functional group transformation - Reagents for the inter conversion of various groups - special and specific oxidizing agents, reducing agents and organo metallic compounds for the inter conversions - the survey of reactions and reagents - Gilman's reagent - LDA - DCC - Wilkinson's catalyst - DDQ - AS - PTS - AP - SeO_2 - Zeolites

Unit - III: Aromatic character and Aromatic substitution reactions

Concepts of aromaticity - Reactions or aromatic compounds - Aromatic electrophilic and nucleophilic substitution reactions - substituent effects on aromatic substitution reactions.

Unit - IV: Synthesis and Reactions of Acetal

Methods of preparation of acetal - mechanism of acetal formation - stability of aliphatic and aromatic acetals and their derivatives - Reaction of acetal with AS, AP, Zeolites etc - Oxidation of ether by various oxidation agents.

Unit - V: Instrumental Techniques

Spectrometric methods for determining the structure of Acetal and their derivatives - FT-IR, NMR, and Mass - Methods of purification, separation-principles of Paper, TLC, Column, HPLC and gas chromatographic techniques-Microwave assisted reactions of acetal

Text Books

1. March J. 1992, Advance Organic Chemistry (Fourth Edition), New York, John-Wiley & Sons.
2. Gould E S. 1959, Mechanism and Structure in Organic Chemistry, New York, Holt-Reinhart and Winston

References

1. Warren S. 1988, Organic Synthesis: The disconnection Approach. New York, John-Wiley.
2. Pine SH etal., 1986, Orgnaic chemistry, Fourth edition, Sigapore, McGraw Hill Book company.

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