

## CH 601: Research Methodology

### UNIT - I

[14 hrs]

Scope of research in chemistry, types of research - basic and applied, frontier areas of research in chemistry, interdisciplinary research, outstanding discoveries and Noble prizes in chemistry during the last two decades. Choosing problem for research consistent with fields of research interests of the students and guide-literature study by a systematic reference work involving the use of books, monographs, periodicals, abstracts, documents, reviews, reports, conference proceedings, patents and dissertations, under the supervision of guide - on-line acquisition of literature (e-journals)

### UNIT - II

[14 hrs]

Research Problem- Identification, statement of research problem, objectives, design and execution of experiments, collection and interpretation of experimental data, arriving at conclusions. Reporting the results of research - style and format - title, abstract, the text, references, tables, figures, elucidations, quotations and footnote. Writing of research papers and dissertations.

### UNIT - III

[14 hrs]

Errors and analysis of experimental data - classification of errors - errors in observation, accidental and systematic errors. Significant figures and computation, statistical treatment of errors - curve fitting and regression analysis - tests of statistical significance 7 hrs.

General awareness of computer hardware, CPU, computer memory, I/O devices, information storage, software components, Types of computers, application of computers, programming languages, computer programs, stored program concept, operating systems, DOS and its use, Algorithm, program flow charts. 7 hrs.

### UNIT - IV

[14 hrs]

#### Introduction to computer applications and programming in chemistry

Applications of computers in chemistry, Programming examples and use of software packages in chemistry 6 hrs.

Chemical Education: Popularization of science education. Social and educational applications of chemical knowledge. 4 hrs.

The changing face of chemistry: Identification and development of key concepts in chemistry. Preparation of audio-visuals for teaching chemistry 4 hrs.

#### Reference:

1. Anderson, Durston and Poole, Thesis and Assignment Writing, Wiley Eastern, 1977
2. A.M. Heiss: Challenge to graduate students, Jossey Bass Inc.
3. J. Topping: Errors of observation and their treatment, Chapman and Hall (1972)
4. I.N. Gibra: Probability and Statistical inference for scientist, prentice Hall (1973)
5. K.V.Raman: Computer in chemistry, TMH N. Delhi (1993)
6. P.N. Arora: Programming with basic for computers, Chand and Co., N. Delhi (1987)
7. Ramkumar: Programming with Fortran - 77 Tata - McGraw Hill, New Delhi (1989)
8. V. Rajaraman: Computer Programming in Fortran IV, V. Prentice Hall. N. Delhi (1987)
9. Chemical Abstracts, Monographs and Internet Services.

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## CH 602: Theoretical Foundations in Chemistry

### Unit - I: Molecular Symmetry and Group Theory:

Molecular Symmetry - symmetry elements and operations.  
Group theory - Concept of a group, definition of point group. Classification of molecules.  
Group multiplication tables. Matrix representations of symmetry operations, class  
similarity transformation, reducible and irreducible representations. The great  
Orthogonality theorem. Character tables, relationship between representations and wave  
functions. Group theory and hybrid orbitals. Group theory and MO's. Molecular  
vibrations - Symmetry types of normal modes of vibrations. Selection rules for  
fundamental vibrational transitions, symmetry considerations to determine IR active and  
Raman active lines. [7 hrs]

**Infrared and Raman Spectroscopy** - Theories and instrumentation, Stretching and  
bending vibrations, Characteristic group frequencies and their dependence on chemical  
environment. **UV and Visible Spectroscopy** - Principles, instrumentation and  
applications. 7 hrs.

### UNIT - II

**Resonance Spectroscopy: Nuclear Magnetic resonance** - Principles and applications in  
structure elucidations. Instrumentation, FT NMR, EPR and its applications. 5 Hrs.  
**Electron spin resonance** - Principles, instrumentation and sampling. ESR of organic free  
radicals in solution, inorganic radicals and transition metals. 3 Hrs.  
**Mass Spectrometry** - Principles, instrumentation, interpretation of mass spectra,  
fragmentation processes. Techniques of ionization, Maldi mass. 2 Hrs.  
**Chromatographic Methods: Principles and applications of column, paper, thin layer  
chromatographic techniques. HPLC, GC, GCMS and LCMS** 2 Hrs.  
**Thermal Analysis** - TG, DTA and DSC - Principles and applications 2 Hrs.

### UNIT - III:

Composite problems involving the applications of UV, IR, proton and C-13 NMR and  
mass spectroscopic techniques. Structural elucidation of organic molecules. 6 Hrs.  
**Reagents and Reaction Mechanisms: Classification of reagent and reactions,**  
nucleophilic, electrophilic substitution reactions, Reactions involving carbonium ions.  
Carbanions, free radicals, carbenes and nitrenes. Methods of determining reaction  
mechanisms, kinetic and non-kinetic methods, mechanisms of oxidation - reduction  
reactions and some important named reactions in organic chemistry 5 Hrs.  
**Asymmetric Synthesis: The chiral pool,  $\alpha$ -amino acids in the synthesis of  
benzodiazepines, carbohydrates, preparation of tomoial from D-mannitol, Felion-Ahn  
model and Cram's chelation control** 3 hrs.

### UNIT - IV: Thermodynamics, Kinetics and Catalysis

Entropy and Free energy concepts, concepts and terminology in kinetics, time scales.  
techniques of measurements of concentrations - conventional and fast techniques.  
Empirical rate equations - methods of determining rate laws. Transition state theory and its  
application to reactions in solution. Activation parameters and their uses. Potential Energy  
surfaces and their applications. Effect of substituents, LFER, kinetic isotopic effect.  
Homogeneous & heterogeneous catalysis-mechanism of surface reactions. [14 hrs]

REFERENCES:



1. V. Ramkrishnan and M.S. Gopinathan: Group theory in Chemistry, Vishal (1988)
2. F. A. Cotton: Chemical Applications of Group theory, Wiley, New York (1993)
3. C. N. Banwell: Fundamentals of Molecular Spectroscopy, Tata McGraw Hill, 1997
4. Willard, Meritt and Dean: Instrumental Methods of Analysis, McGraw Hill (1993)
5. R. S. Drago: Physical Methods in Inorganic Chemistry, Affiliated East-West (1977)
6. P. S. Kalsi: Organic Spectroscopy, Wiley Eastern New Delhi (1990)
7. F. W. McLafferty, W.A. Benjamin Meulo: Interpretation of Mass Spectroscopy, 2<sup>nd</sup> ed
8. R. M. Silverstein, G.C. Bassler and T.C. Morrill: Spectrometric Identification of Organic Compound, Wiley (1991)
9. W. Kemp: Organic Spectroscopy, ELBS, Mac Millan (1991)
10. E. A. Edsworth, David W.H. Rankin and Stephen Cradock: Structural Methods in Inorganic Chemistry, Blackwell Scientific Publications, London, (1991)
11. D.A. Skoog and D.M. West: Principles of Instrumental Analysis, Saunders (1980)
12. Concepts and Models in Inorganic Chemistry- Douglas, Alexander & McDaniel, Wiley (2001).
13. Comprehensive Inorganic Chemistry – Ed. J C Bailar, Pergamon Press, 1982
14. Advanced Organic Chemistry – J March , Wiley
15. Stereochemistry of Organic Compounds – Nasipuri, New Age International.
16. Organic Chemistry – Clayden, Greeves, Warren & P Wothers – Oxford Univ. Press.

### CH 611: Coordination Chemistry

UNIT-I: [14 hrs]  
 Synthesis, Purification and Characterization of Coordination Compounds: Metal aqua ions, solvents and ionic liquids, chromatographic methods, crystal growth methods. Newer methods of synthesis- solid state methods, sol-gel, sonochemistry, microwave assemblies and self-assembly and electrochemical, supramolecular systems.

UNIT-II: [14 hrs]  
 Physical Methods of Characterization- Case Studies: NMR, ESR, ENDOR, XRD, Raman and FT-IR. Resonance Raman, Photoelectron, Mossbauer, Electrochemical, Optical, MCD, Mass. Solvatochromism, Electronic spin cross-over.

UNIT-III: [14 hrs]  
 Bio-coordination Chemistry: Electron transfer systems- cytochromes, iron-sulphur proteins, cuprodoxins. Ion recognition and Transport. Dioxygen-binding proteins, heme-peroxidases, copper oxidases. nitrogen fixation, zinc hydrolases, bioorganometallic chemistry of Co & Ni.

UNIT-IV: [14 hrs]  
 Applications: Catalysis- polymerization, hydrogenation, CO addition, C-C cross coupling, C-heteroatom cross coupling. Lewis acid catalysts, supported metal catalysts, biomedical applications.

#### Reference:

1. Comprehensive Coordination Chemistry -J.A. McCleverty & T J Meyer Elsevier (2004)
2. Comprehensive Coordination Chemistry, Ed. G Wilkinson, Pergamon (1984)

## CH 612: Analytical and Structural Chemistry

### UNIT – I: Analytical Techniques

[14 hrs].

**Introduction:** General Description of chromatography, migration rates of solutes. Band broadening, column efficiency and resolution. **Ion exchange chromatography:** Structures of resins, selectivity, capacity of resins, removal of interfering ions, concentration and recovery of trace metals, anion and cation separations and application for the separation of lanthanides and actinides. Techniques of column chromatography, size exclusion chromatography. **Gas Chromatography:** Principles, columns and detectors.

### UNIT – II:

[14 hrs].

**HPLC:** Principles, equipment, columns, detectors, choice of column, materials. **Paper chromatography:** Theory and principle. Techniques; one, two- dimensional and circular paper chromatography and applications.

**TLC:** Efficiency of TL plates, selection of stationary & mobile phases

**AAS:** Theory, working of AAS instruments, analytical applications, interferences.

**Emission Spectroscopy:** Flame Emission Spectroscopy, plasma emission spectrometry. Principles of flame photometry, evaluation methods in flame photometry, interferences.

**Molecular Luminescence Spectroscopy:** Theory of fluorescence and phosphorescence fluorimetry in quantitative analysis, instruments, fluorescence and structure, fluorescence quenching, phosphorescence method, applications in quantitative analysis.

### UNIT – III:

[14 hrs].

**Light-Scattering methods:** Nephelometry & turbidimetry-theory, effects of concentration, particle size & wavelength on scattering, instrumentation & application. **Activation analysis**

**Thermal methods:** Thermogravimetric analysis, instrumentation, factors affecting the results and applications. **Differential thermal analysis,** simultaneous DTA-TGA curves. **Differential scanning calorimetry,** applications.

**Electrophoresis:** Theory and classification. Factors influencing mobility, macromolecular size and charge, interaction with supporting electrolyte, pH and concentration discontinuities. Factors affecting electrophoretic phenomena, electrolysis, electroosmosis, temperature and supporting media. Instrumentation and methodology.

### UNIT – IV

[14 hrs].

**The Crystal Structure Studies:** Diffraction of X-Rays by Crystals, Stages of X-Ray Structure Analysis of Single Crystals. X-Ray Diffractometers for Investigating Single Crystals. Determination of the Crystal Orientation, Unit Cell and Intensities, Characterisation and Data Collection, Structure Solution and Structure Refinement – SHELXS, SHELXL and other programmes, Calculation of Molecular Parameters, Graphical Visualisation, Plotting and other Analysis, Document Preparation and Word Processing, An introduction to packing of molecules in the crystal structures and Hydrogen Bonding. An introduction to powder diffraction.

### REFERENCES :

1. G.D. Christian : Analytical Chemistry, (4th Ed.), (John Wiley ), 1986.
2. R.A. Day and A.L. Underwood : Quantitative Analysis, 5<sup>th</sup> Ed. (Prentice Hall, India), 1998.
3. H.H. Willard, L.L. Merrit and J.J. Dean, Instrumental methods of analysis, (7<sup>th</sup> Ed.) 1988
4. B.K. Sharma, Instrumental methods of chemical analysis, Goel publishing House, 2000.
5. Skoog, Holler and Nieman: Principles of Instrumental Analysis, Harcourt Afea, 2001
6. Structural Methods in Inorganic Chemistry, Vol I & II, E.A.V. Ebsworth, D.W.H. Ranklin & S. Craddock, Blackwell Scientific, 1991.
7. A K Tareen and Kuty, Crystallography, University Press, 2002.
8. F.C. Ladd Mark & Palmer, R.A : Structure Determination by X-Ray Crystallography, 2003.



CH 621: Heterocyclic and Medicinal Chemistry

UNIT - I

**Nomenclature of Heterocyclic Compounds:** Trivial or traditional names, Early semisystematic convention and Hantzsch - Widman system. [14 hrs]

**Nomenclature of polycyclic systems:** Trivial names, IUPAC names, Fusion names, Bridged and fused structures, von-Baeyer names, Spiro names and naming of cyclophanes.

**Interconversion of Heterocycles and Rearrangements of heterocyclic compounds:** Reactions involving interconversion of heterocycles such as furan to pyrazole. Pyrazole to pyridine, Isatin to Quinoline, Isatogens, Quinazolones and Cinnolines. Rearrangements and ring transformation of 1,2,3-Triazoles, Oxazoles, 1,2,3-Oxadiazoles, Pyridazines, Quinoxalines and Quinoxalin - N-Oxides.

UNIT - II

A few typical examples of synthesis of non-heterocycles employing isoxazoles, thiazoles, pyran and pyridine derivatives. [14 hrs]

**Photochemistry of Heterocycles:** Photo-oxidation of pyrroles, photochemical reactions of pyrazoles, 1,2,3 and 1,2,4-triazoles, 1,2,3-triazines, 1,3,4-oxadiazoles, mono and disubstituted tetrazoles. Photochemistry of pyridazines and pyrimidines.

UNIT - III

Concept of prodrugs, analogues, concept of lead molecules, in drug design, factors governing drug design. Drug design through molecular disjunction and through molecular conjugation. Tailoring of drugs through the application of principles of Bio-isosterism. Structurally specific and non-specific drugs, factors responsible for drug reaching the active site. Thermodynamic activity, Meyer-Overton and Ferguson Theory. Biochemical and Physiological information leading to the development of new drugs. Quantitative analysis of SAR, Fundamentals of QSAR, Objectives of QSAR. Expression of biological activity, parameters related to chemical structure. Hanch analysis & its application in Medicinal Chemistry. Steric feature of drugs, optical isomerism and biological activity. [14 hrs]

UNIT - IV

A detailed discussion including classification, synthesis, test for identification and methods of assay of the following class of drugs. Antipsychotic agents, Anxiolytics. Drugs used in hyperkinetic disorders. Hypertensive drugs, Cardiovascular drugs. Antineoplastic agents and Antiviral agents. [14 hrs]

References

1. Text book of Medicinal Chemistry by Burger.
2. Text book of Medicinal Chemistry by Wilson & Gisvold
3. Principles of Medicinal Chemistry- William O Poye
4. Medicinal Chemistry- Ashuthosh Kar
5. J.A.Joule and G.F.Smith: Heterocyclic Chemistry, Cambridge University press (1972).
6. A.R.Katritzky and C.J.Rees: Comprehensive Heterocyclic Chemistry, Pergamon (1984).
7. D.H.R.Barton and W.D.Ollis: Comprehensive Organic Chemistry, Vol 14, Heterocyclic Compounds, Pergamon (1979)
8. A.R.Katritzky: Advances in Heterocyclic Chemistry, Vol 15-25, Academic (1971-81)



[14 hrs]

## UNIT - I

**Principles of Reactivity:** An overview of kinetic concepts and analysis of kinetic results - rates of simple and composite chemical reactions (simultaneous and consecutive), steady-state treatment, empirical rate equations, methods of determining rate laws. Transition state theory, its limitations and extensions. Applications to reactions in solution. Activation parameters from experimental results, mechanistic significance and their uses. General approaches to reaction mechanism- kinetic & thermodynamic control of reactions. Reactivity-selectivity principles (Hammond's & Curtin-Hammett postulates). 10 Hrs.

**Fast Reaction Techniques:** Flow, flash photolysis, relaxation and NMR methods. A brief molecular beam studies of reactive collision. Kinetic spectroscopy. 4 Hrs.

[14 hrs]

## UNIT - II

**Potential energy surfaces:** - Features & construction. Theoretical calculation of  $E_a$ . Tunneling effect. Isotope effects with heavier atoms. 5 Hrs.

**Theory of kinetic isotope effects** - Primary, secondary and solvent kinetic isotope effects. Substituent Effects on Reactivity: Inductive effect, electromeric effect, substitutions and the energy of activation. Hammett & Taft equations, LFERs, Deviations from Hammett equation. Dual-parameter correlations-  $\sigma_1$ - &  $\sigma_R$ - scales: Swain-Scott & Edward equations, Winstein Grunwald relationship, Isokinetic relationship. 5 Hrs.

**Solvation and Solvent Effects:** Cage effect, effects of ionic strength, dielectric constant and solvation on rates of reactions (ion-ion, ion-dipole & dipole-dipole reactions) 4 Hrs.

[14 hrs]

## UNIT - III

**Homogeneous catalysis:** Electronic and structural effects on acidity and basicity. Acidity functions - Hammett acidity function and its applications. Industrial catalysts: catalyst carrier, promoter, inhibitor & catalyst poison. 4 Hrs.

**Reactions at Surfaces:** Mechanisms of surface reactions- kinetic effects of surface heterogeneity & interactions - surface inhibition and activation energies - surface exchange reactions- TST of surface reactions- unimolecular & bimolecular reactions. 5 hrs.

**Micelles:** Surface active agents- micellisation, CMC, micellar catalysis.

**Pharmaco kinetics:** Pharma concentration time curve, protein binding and drugs, drug dissolution rate, pharmacokinetics applied to one-component open model (calculation of elimination rate constant & metabolism constant). 5 hrs.

[14 hrs]

## UNIT - IV

**The Crystal Structure Studies:** Diffraction of X-Rays by Crystals, Stages of X-Ray Structure Analysis of Single Crystals, X-Ray Diffractometers for Investigating Single Crystals. Determination of Crystal Orientation, Unit Cell and Intensities, Characterisation and Data Collection, Structure Solution and Structure Refinement - SHELXS, SHELXL and other programmes, Calculation of Molecular Parameters, Graphical Visualisation, Plotting and other Analysis. Document Preparation and Word Processing. An Introduction to packing of molecules in the crystal structures and Hydrogen Bonding. An introduction to powder diffraction.

## REFERENCES :

1. Physical Chemistry, 5<sup>th</sup> ed., - Atkins (ELBS) 1995
2. Chemical Kinetics - K.J.Laidler (Pearson Education) 1987.
3. The Physical Basis of Organic Chemistry, H.Maskill, Oxford University Press.

## CH 633: Polymer Chemistry

### Unit I

Conventional and specialized methods of polymer preparation: -Details of free radical, ionic and coordination polymerization considering the examples of common industrial polymers. Few new specialized techniques -- Metathesis, Group transfer polymerization etc.  
Chemical modification of polymers. 14 hrs

### Unit II

Properties and behaviour of polymers-solid state properties and behaviour of polymers in solution. Techniques of Analysis and Characterization-Physical, Analytical, microscopic and spectroscopic methods of characterization. 14 hrs

### Unit III

Engineering and Specialty polymers: Blends, composites, IPN systems, conducting polymers, liquid crystalline polymers: Structural requirements, Preparation, Properties and applications. 14 hrs

### Unit IV

Degradation and stability. Modes of Degradation, Polymer waste disposal techniques. Biodegradable plastics. Pharmaceutical and Medical Applications of polymers. 14 hrs

### REFERENCES :

1. Text book of Polymer Science : F.W. Billmeyer ( Wiley)
2. Contemporary Polymer Chemistry-H.R.Alcock and F.W.Lampe (Prentice Hall)
3. Polymer Science:V.R.Gowariker, N.V.Viswanathan & T.Sreedhar(Wiley Eastern)
4. Polymer science and Technology, J.R.Fried (Prentice Hall).





ಮಂಗಳೂರು



ವಿಶ್ವವಿದ್ಯಾನಿಲಯ

ಕುಲಸಚಿವರ ಕಛೇರಿ

ಮಂಗಳಗಂಗೋತ್ರಿ - 574199

ಸಂಖ್ಯೆ: ಮಂವಿ/ಶೈಕ್ಷಣಿಕ/ಸಿಆರ್.14/2011-12/ಎ2/1061

ದಿನಾಂಕ: 28.01.2015

ರಿಗೆ:

ಸಂಯೋಜಕರು,  
ಎಂ.ಎಸ್ಸಿ. ಕೈಗಾರಿಕಾ ರಸಾಯನಶಾಸ್ತ್ರ,  
ಮಂಗಳೂರು ವಿಶ್ವವಿದ್ಯಾನಿಲಯ,

ಮಾನ್ಯರೇ,

ವಿಷಯ: ಕೈಗಾರಿಕಾ ರಸಾಯನಶಾಸ್ತ್ರ ಪಿಹೆಚ್.ಡಿ. ಪದವಿಯ ಕೋರ್ಸುಗಳಿಗೆ ಪಠ್ಯಕ್ರಮವನ್ನು  
ಅಳವಡಿಸುವ ಬಗ್ಗೆ

ಉಲ್ಲೇಖ: 1) ದಿನಾಂಕ 20.09.2014ರಂದು ನಡೆದ ಸ್ನಾತಕೋತ್ತರ ಕೈಗಾರಿಕಾ ರಸಾಯನಶಾಸ್ತ್ರ  
ಅಧ್ಯಯನ ಮಂಡಳಿ ಸಭೆಯ ನಿರ್ಣಯ

2) ತಮ್ಮ ಪತ್ರ ಸಂಖ್ಯೆ: MU/IND-CHEM/Ph.D/ADM-01/2014-15/849,  
ದಿನಾಂಕ 23.12.2014

ಮೇಲಿನ ವಿಷಯಕ್ಕೆ ಸಂಬಂಧಿಸಿದಂತೆ, ಉಲ್ಲೇಖ (1)ರಲ್ಲಿ ತಿಳಿಸಲಾದ ಸಭೆಯಲ್ಲಿ ನಿರ್ಣಯವಾದಂತೆ  
ಕೈಗಾರಿಕಾ ರಸಾಯನ ಶಾಸ್ತ್ರ ಪಿಹೆಚ್.ಡಿ. ಪದವಿಯ ಕೋರ್ಸುಗಳಿಗೆ ರಸಾಯನಶಾಸ್ತ್ರ ಪಿಹೆಚ್.ಡಿ. ಪದವಿಯ  
ಕೋರ್ಸುಗಳಿಗೆ ಪಠ್ಯಕ್ರಮವನ್ನು ಶೈಕ್ಷಣಿಕ ವರ್ಷ 2015-16ನೇ ಸಾಲಿನಲ್ಲಿ ಮಾತ್ರ ಅಳವಡಿಸಿಕೊಳ್ಳಲು ಈ  
ಮೂಲಕ ಅನುಮತಿ ನೀಡಲಾಗಿದೆ.

ಮುಂದಿನ ಶೈಕ್ಷಣಿಕ ವರ್ಷದಲ್ಲಿ ಸದರಿ ಪದವಿಗೆ ಪ್ರತ್ಯೇಕವಾಗಿ ಪಠ್ಯಕ್ರಮವನ್ನು ತಯಾರಿಸಲು  
ತಿಳಿಸಲಾಗಿದೆ.

ತಮ್ಮ ವಿಶ್ವಾಸಿ,

ಕುಲಸಚಿವರು  
K.L.V.

Ph.D. file  
Ph.D. file  
21/1/15