

Mangalore University  
**Department of Studies in Chemistry**

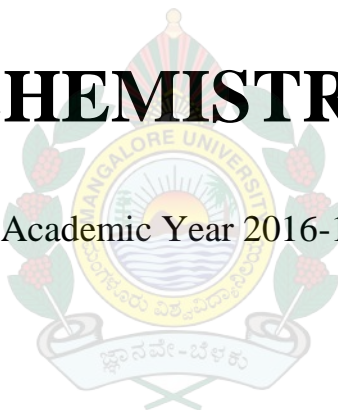
**M. Sc. Degree Programmes**

**(CHOICE BASED CREDIT SYSTEM – SEMESTER SCHEME)**

**Syllabi for M.Sc., Courses in**

**CHEMISTRY**

(From the Academic Year 2016-17 onwards)



**Mangalore University**  
**M. Sc. Degree Programme in Chemistry:**

**CHOICE BASED CREDIT SYSTEM (CBCS) SEMESTER SCHEME**

**COURSE PATTERN AND SCHEME OF EXAMINATION**

(Year 2016-2017 onwards)

**PREAMBLE**

Revision of Syllabi for the Two years Master Degree (Choice Based Credit System-Semester Scheme) Programmes in Chemistry, Applied Chemistry, Organic Chemistry and Analytical Chemistry.

PG BOS in Chemistry has revised and prepared the Syllabi (CBCS based) for all the Four Courses -Chemistry, Applied Chemistry, Organic Chemistry and Analytical Chemistry in its meeting held on 24<sup>th</sup> July 2014 and the University implemented it from the same academic year. Now the University has asked the PG BOS in Chemistry to revise the syllabi by giving certain Guidelines (Ref:-No: MU/ACC/CR.38/ CBCS (PG)/2015-16 dt.05-05-2016 bse on UGC letter) for all the four Courses (Programmes) to offer Hard Core, Soft Core and Open Elective courses with credits to each course amounting to 92 credits for the entire programme.

Accordingly, the PG BOS in Chemistry prepared the syllabi for all the four programmes. It has prepared course pattern by proposing 12 Hard Core theory courses (3 in each semester) and 5 practical courses (in 3<sup>rd</sup> and 4<sup>th</sup> semester), one Project work (in 4<sup>th</sup> Semester with 4 credits) with a provision to have One Project Work in lieu of one of the practicals in 4<sup>th</sup> semester in each programme with 3 credits each (project work - 4 credits) with total of **55 Credits**. BOS is offering 3, 2, 2 and 3 (Total 10 courses) Soft core courses respectively in 1<sup>st</sup>, 2<sup>nd</sup>, 3<sup>rd</sup> and 4<sup>th</sup> semesters of a programme. Student shall opt any 2, 1, 1 and 2 (Total 6 courses) courses respectively in 1<sup>st</sup>, 2<sup>nd</sup>, 3<sup>rd</sup>, 4<sup>th</sup> Semesters. All the soft core courses are of 3 credits. Programme consists of 6 Soft Core practical courses (3 courses each in 1<sup>st</sup> and 2<sup>nd</sup> semesters of the Programme with 2 credits each) with a total of **30 credits** (6 theory x 3 credits + 6 practicals x 2 credits). BOS has also proposed 2 open electives (1 each in 2<sup>nd</sup> & 3<sup>rd</sup> Semesters of the programme) with 3 credits each (**6 credits**). All together **total credits** come to 91 from teaching. I have prepared a draft course pattern by considering all the points mentioned in the above said letter from the Registrar and placing it before the BOS meeting.

Detailed syllabi for 1<sup>st</sup> and 2<sup>nd</sup> Semesters are prepared and enclosed, whereas the syllabi for the 3<sup>rd</sup> and 4<sup>th</sup> Semesters will be prepared in forthcoming BOS meeting.

### Course/credit pattern:

Semester Credits	Hard Core(H)(T)	Soft Core (S)(T)	Elective E)(T)	Practical	Tutorial	Total Credits
First	9	6	--	6 (S)	--	21
Second	9	3	3	6 (S)	--	21
Third	9	3	3	9 (H)	--	24
Fourth	9	6	--	10(H)	--	25
Total	36	18	6*	12(S) + 19(H)	--	91

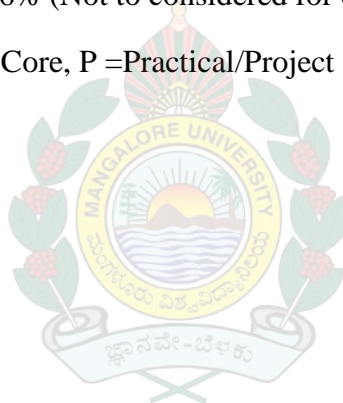
Total Credits from all the Four Semesters (1<sup>st</sup>, 2<sup>nd</sup>, 3<sup>rd</sup> and 4<sup>th</sup>) : 21+21+24+25 = 91

Total Hard Core credits = 36 (T) + 19 (P) = 55 = 60.4%

Total Soft Core credits = 18 (T) + 12(P) = 30 = 33.0%

\*Open Elective Credits = 6 = 6.6% (Not to considered for calculating the

CGPA) H= Hard Core, S= Soft Core, P =Practical/Project



**Consolidated Course code and title  
Programme: M.Sc. in Chemistry**

**1<sup>st</sup> Semester**

**2<sup>nd</sup> Semester**

Course Code	Course Title	Course Code	Course Title
CH H 401	Inorganic Chemistry	CH H 451	Advanced Inorganic Chemistry
CH H 402	Organic Chemistry	CH H 452	Advanced Organic Chemistry
CH H 403	Physical Chemistry	CH H 453	Advanced Physical Chemistry
CH S 404 Or CH S 405	Inorganic Spectroscopy and Analytical Techniques Or Environmental Chemistry	CH S 454 Or CH S 455	Organic Spectroscopic Techniques Or Chemistry of Bio-molecules
CH S 406	Molecular Spectroscopy and Diffraction Techniques	CH E 456	Environmental, Electro- and Polymer Chemistry
CH P 407	Inorganic Chemistry Practicals-1	CH P 457	Inorganic Chemistry Practicals-II
CH P 408	Organic Chemistry Practicals-1	CH P 458	Organic Chemistry Practicals-II
CH P 409	Physical Chemistry Practicals-1	CH P 459	Physical Chemistry Practicals-II

**3<sup>rd</sup> Semester**

**4<sup>th</sup> Semester**

CH H 501	Coordination Chemistry	CH H 551	Bioinorganic Chemistry
CH H 502	Organic Reaction Mechanism and Heterocyclic Chemistry	CH H 552	Organic Synthetic Methods
CH H 503	Solid State Chemistry	CH H 553	Electrochemistry and Reaction Dynamics
CH S 504 Or CH S 505	Medicinal & Natural Product Chemistry Or Bioorganic Chemistry	CH S 554	Organometallic Chemistry
CH E 506	Analytical and Green Chemistry	CH S 555 Or CH S 556	Polymer Chemistry Or Nuclear, Radiation & Photochemistry
CH P 507	Inorganic Chemistry Practicals-III	CH P 557	Inorganic Chemistry Practicals-IV
CH P 508	Organic Chemistry Practicals-III	CH P 558	Physical Chemistry Practicals-IV
CH P 509	Physical Chemistry Practicals-III	CH P 559	Project Work & Dissertation

**Detailed distribution of Course & Credits:**Programme: **Chemistry:****1<sup>st</sup> Semester**

Course Code	Course Title	No of UNITs	Evaluation IA + Exam	Teaching hr week Sem	Exam Hrs	Credits
CH H 401	Inorganic Chemistry	3	30 + 70	3 45	3	3
CH H 402	Organic Chemistry	3	30 + 70	3 45	3	3
CH H 403	Physical Chemistry	3	30 + 70	3 45	3	3
CH S 404 Or CH S 405	Inorganic Spectroscopy and Analytical Techniques Or Environmental Chemistry	3 3	30 + 70 30 + 70	3 36 3 36	3	3
CH S 406	Molecular Spectroscopy and Diffraction Techniques	3	30 + 70	3 36	3	3
CH P 407	Inorganic Chemistry Practicals-1	4 Hrs	30 + 70	4	4	2
CH P 408	Organic Chemistry Practicals-1	4 Hrs	30 + 70	4	4	2
CH P 409	Physical Chemistry Practicals-1	4 Hrs	30 + 70	4	4	2

Total credits from 1<sup>st</sup> Semester: **21** (Hard Core-9, Soft Core-12)**2<sup>nd</sup> Semester**

Course Code	Course Title	No of UNITs	Evaluation IA+ Exam	Teaching hr week Sem	Exam Hrs	Credits
CH H 451	Advanced Inorganic Chemistry	3	30 + 70	3 45	3	3
CH H 452	Advanced Organic Chemistry	3	30 + 70	3 45	3	3
CH H 453	Advanced Physical Chemistry	3	30 + 70	3 45	3	3
CH S 454 Or CH S 455	Organic Spectroscopic Techniques Or Chemistry of Bio-molecules	3 3	30+70 30 + 70	3 36 3 36	3	3
CH E 456	Environmental, Electro- and Surface Chemistry	3	30 + 70	3 36	3	3
CH P 457	Inorganic Chemistry Practicals-II	4 Hrs	30 + 70	4	4	2
CH P 458	Organic Chemistry Practicals-II	4 Hrs	30 + 70	4	4	2
CH P 459	Physical Chemistry Practicals-II	4 Hrs	30 + 70	4	4	2

### 3<sup>rd</sup> Semester

Course Code	Course Title	No of UNITS	Evaluation IA +Exam	Teaching hr week	Sem	Exam Hrs	Credits
CH H 501	Coordination Chemistry	3	30 + 70	3	45	3	3
CH H 502	Organic Reaction Mechanism and Heterocyclic Chemistry	3	30 + 70	3	45	3	3
CH H 503	Solid State Chemistry	3	30 + 70	3	45	3	3
CH S 504 Or CH S 505	Medicinal & Natural Product Chemistry Or Bioorganic Chemistry	3 3	30 + 70 30 + 70	3 3	36 36	3	3
CH E 506	Analytical & Green Chemistry	3	30 + 70	3	36	3	3
CH P 507	Inorganic Chemistry Practicals-III	6 Hrs	30 + 70	6		6	3
CH P 508	Organic Chemistry Practicals-III	6 Hrs	30 + 70	6		6	3
CH P 509	Physical Chemistry Practicals-III	6 Hrs	30 + 70	6		6	3

Total Credits = **24** (Hard Core-18, Soft Core-3 and Elective-3)

### 4<sup>th</sup> Semester

Course Code	Course Title	No of UNITS	Evaluation IA + Exam	Teaching hr week	Sem	Exam hrs	Credits
CH H 551	Bioinorganic Chemistry	3	30 + 70	3	45	3	3
CH H 552	Organic Synthetic Methods	3	30 + 70	3	45	3	3
CH H 553	Electrochemistry and Reaction Dynamics	3	30 + 70	3	45	3	3
CH S 554	Organ metallic Chemistry	3	30 + 70	3	36	3	3
CH S 555 Or CH S 556	Polymer Chemistry Or Nuclear, Radiation & Photochemistry	3 3	30 + 70 30 + 70	3 3	36 36	3	3
CH P 557	Inorganic Chemistry Practicals -IV	6 Hrs	30 + 70	6		6	3
CH P 558	Physical Chemistry Practicals -IV	6 Hrs	30 + 70	6		6	3
CH P 559	Project Work & Dissertation	8 Hrs	30 + 70	8		--	4

Total Credits = **25** (Hard Core-18, Soft Core-6 + Seminar- 1)

**Total Credits: 21+21+24+25 = 91.**

## Question Paper Setting:

**A. BASIS FOR INTERNAL ASSESSMENT:** Internal assessment marks in theory papers shall be based on two tests. The tests may be conducted 8 and 14 weeks after the start of a semester. Average of two test marks will be considered as internal assessment marks. Practical internal assessment marks shall be based on test and records. 20 marks for experiment and 10 marks for record. The practical tests may be conducted 12 weeks after the start of a semester. Internal Assessment marks on Project work-Dissertation is based on two seminars of 45 minutes duration each carrying 15 marks. The Seminar is to be delivered in 3<sup>rd</sup> semester on the subject and 4<sup>th</sup> semester on their project work.

**B. THEORY QUESTION PAPERS PATTERN:** The Syllabus of each hard core course shall be grouped into three UNITS of 15 teaching hours and that of soft core and open Elective shall be of three UNITS of 12 teaching hours. Question Papers in all the four semesters shall consist of Two Parts- Part A and Part-B. Part A shall contain Nine (09) very short answer objective type questions carrying 2 marks each, drawn equally from all the three UNITS of the syllabus. All the nine subdivisions are to be answered. Part B shall contain Six (06) brief and/or long answer questions carrying 13 marks each drawn from all the three UNITS of the syllabus (2 questions per UNIT). There may be a maximum of three sub-divisions per question, carrying 3 or more marks per sub-division. Four (04) out of Six (06) questions are to be answered.

**C. PRACTICAL EXAMINATION PATTERN:** Practical Examination course papers out of 70 marks 15 marks shall be allotted for Viva voce and 55 marks for practical proper. In the 4<sup>th</sup> semester there shall project work/dissertation in lieu of one of the practicals for all the programmes (Chemistry, Applied Chemistry, Organic Chemistry and Analytical Chemistry) consisting of 70 marks. The Project work may be conducted either in the department or in an Institution or Industry. Project report shall be valued for 70 marks.

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## OBJECTIVES OF THE SYLLABUS

The revised syllabus is designed to provide a flexible structure within which students can choose the topic of their interest in addition to a specific knowledge. The syllabus takes into account the requirements for higher education to improve the quality of education and student competency level on par with national and international institutions. The syllabus is structured in such a way so as to ensure that students become aware of the practical applications of scientific knowledge to build careers in the scientific field.

The syllabus aims to enable students to:

- Prepare the students for employment and for further studies by acquiring the knowledge and understanding of chemical principles.
- Appreciate, understand and use the scientific method in the solving of problems. Develop the ability to disseminate chemical information effectively.
- Acquire good laboratory skills and practice safety measures when using equipment and chemicals as well as the safe disposal of chemical waste.
- Apply chemical knowledge to everyday life situations and develop inquisitiveness in order to continue the search for new ways in which the resources of our environment can be used in a sustainable way.

## PROGRAMME OUTCOMES

- Master of Science in Chemistry basically aims at the training of students with a detailed knowledge base in Chemistry of potential utility in academia as well as Industry through advanced course work and laboratory work in the department and a project work in industries or premier institutions.
- To qualify NET/GATE/SET/Civil Services and other competitive examinations.
- For exploring global level research opportunities for doctoral and post-doctoral studies.
- For professional employment in different domains such as academics, industries, analytical laboratories, scientific organizations, entrepreneurship, administrative positions etc.
- For enhancing the connectivity between academic and industrial institutions.

## PROGRAMME SPECIFIC OUTCOMES

- Students will equip themselves with up-to-date knowledge in the field of frontier areas of chemistry.
- Attain confidence to take up R & D positions in teaching, higher education institutions, public sector & private companies.
- Get motivated to take up higher studies.
- Will be able to use their knowledge in day to day life and work for betterment of society.
- Understand the social responsibility of chemistry in educating general public about protection of environment against pollution.
- Knowledge & Confidence to clear nation level competitive examinations.
- To make use of the chemistry knowledge to analyze real samples like food samples, biological samples, pharmaceutical products and environmental samples.
- To propose/develop most effective and novel methods of synthesis of bioactive compounds/ nanomaterials and in turn to design target oriented drugs to treat different diseases.
- To propose/develop simple and accurate analytical methods as alternatives for the existing standard/official methods for the analysis of complex matrices/clinical samples.
- To develop energy storage materials and fuel cells.



## FIRST SEMESTER

### CH H 401: INORGANIC CHEMISTRY

#### COURSE OUTCOMES:

- Students will learn the basics of ionic and covalent bonding, lattice energy, hydration energy,
- This course enables the students to understand VSEPR theory and MOT theory.
- This course will Enlighten the students to understand Noble gas chemistry, Graphitic compounds, HSAB Concept,
- Theories of redox indicators and sampling techniques.

#### UNIT- I:

[15 Hours]

Ionic bond: Properties of ionic substances, coordination number of an ion, structures of crystal lattices- NaCl, CsCl, ZnS and rutile. Lattice energy- Born Lande equation, Born-Haber cycle, Uses of Born-Haber type of calculations. Ionic radii, methods of determining ionic radii, factors affecting ionic radii, radius ratio rule, covalent character in ionic bonds, hydration energy and solubility of ionic solids.

Covalent bond: valence bond theory, resonance, hybridisation, Bent's rules and energetics of hybridization, Deduction of molecular shapes – VSEPR theory.

M.O.theory, application to homo- and hetero-diatomic and -triatomic molecules.

#### UNIT -II:

[15 Hours]

Alkali and alkaline earth metal complexes of crown ethers, cryptands and calixarenes and their biological significance.

Halogens and Noble gas chemistry –interhalogens, psuedohalogens, polyhalide ions, oxyhalogen species, xenon oxides and fluorides. Oxy- and peroxy acids of N, P and S.

Graphitic compounds, carbides, pure silicon, silica and silicates, zeolites.

HSAB concept. super acids. Reactions in non-aqueous media: Liquid ammonia, anhydrous sulphuric acid, glacial acetic acid, anhydrous HF, bromine trifluoride, liquid sulphur dioxide and dinitrogen tetroxide. Reactions in molten salts.

#### UNIT- III:

[15 Hours]

Precipitation phenomena: precipitation from homogeneous solutions, organic precipitants in inorganic analysis. Solvent extraction of metal ions, nature of extractant, distribution law, partition coefficients, types of extractions and applications.

Theories of redox indicators, titration curves, feasibility of redox titrations.

Chelometric titrations- titration curves with EDTA, feasibility of EDTA titrations, indicators for chelometric titrations, selective masking and demasking techniques, industrial applications of masking.

Sampling techniques, preparation of samples for analysis. Nature of errors, statistical treatment of errors, the t- and F-tests, significant figures, rejection of data.

## REFERENCES:

1. J.E Huheey, Keiter, Keiter and Medhi: Inorganic Chemistry (4th ed.), Pearson Education, 2006.
2. Shriver, Atkins and Langford: Inorganic Chemistry (3<sup>rd</sup>edn.) OUP, 1999.
3. J.D. Lee: Concise Inorganic Chemistry, (5<sup>th</sup>edn.) Blackwell Science, 2000.
4. B.E. Douglas, D. McDaniel & A Alexander: Concepts & Models of Inorganic Chemistry, Wiley 2001
5. W.W. Porterfield: Inorganic chemistry – A Unified Approach, Elsevier, 2005.
6. R.A. Day and A.L. Underwood: Quantitative Analysis, 5<sup>th</sup> Ed. (Prentice Hall, India), 1998.



## CH H 402: ORGANIC CHEMISTRY

### COURSE OUTCOME:

- Enable the students to learn the bonding in organic systems, various aspects of aromaticity, electronic effects, acidity and basicity of organic compounds.
- To gain knowledge on methods of determination of reaction mechanism, various reaction intermediates and aliphatic nucleophilic substitution reactions.
- To understand the detailed aspects of optical and geometrical isomerism.

### UNIT-I:

[15 Hours]

**Bonding in organic systems:** Theories of bonding-Valence and molecular orbital approaches. Resonance, hyper-conjugation and tautomerism, Huckel molecular orbital theory and its application to simple systems- ethylene, allyl, cyclopropyl, butadienyl, cyclopentadienyl, pentadienyl, hexatrienyl, heptatrienyl systems. Calculation of the total energy and M.O. coefficients of the systems. 5 hrs

**Aromaticity:** Concept of aromaticity, Huckel's rule, Polygon rule, Homo-aromatic, non aromatic and anti-aromatic systems. Aromaticity in benzenoid and non-benzenoid molecules. Annulenes & hetero-annulenes. Physical methods to study aromaticity-UV, IR &  $^1\text{H}$  NMR. 4 hrs

**Bonds weaker than covalent:** Addition compounds, crown ether complexes, cryptands, inclusion compounds, catenanes, fluxional molecules. 3 hrs

**Structure and reactivity:** Effects of hydrogen bonding, resonance, inductive and hyperconjugation on strengths of acids and bases. 3 hrs

### UNIT-II:

[15 Hours]

**Methods of Determining Reaction Mechanism:** Kinetic and non-kinetic methods, Identification of products, detection of intermediates, isotopic labelling, stereo chemical evidences, cross-over experiments, Limitation of reactions, kinetic evidences and kinetic isotopic effects. 5 hrs

**Reaction Intermediates:** Generation, structure, stability, reactivity, detection, trapping and reactions of classical and non-classical carbocations, carbanions, free radicals, carbenes, nitrenes and arynes. Singlet oxygen-generation and reactions with organic molecules. 5 hrs

**Aliphatic Nucleophilic Substitution Reactions:** Mechanism and scope of aliphatic nucleophilic substitution reactions- $\text{S}_{\text{N}}1$ ,  $\text{S}_{\text{N}}2$  and  $\text{S}_{\text{N}}\text{i}$ . Stereochemistry of nucleophilic substitution reactions, allylic nucleophilic substitution reactions, Walden inversion, neighbouring group participation & anchimeric assistance. Factors influencing the rates of nucleophilic substitution reactions. 5 hrs

### UNIT-III: Stereochemistry

[15 Hours]

**Optical Isomerism:** Conformation and configuration of molecules, projection formulae, Fischer, Saw-horse, Newman and Flying wedge representations. Interconversion of these formulae. Absolute configuration (D,L) and (R,S) systems. Elements of symmetry, Pseudoasymmetric centres, chirality, molecules with more than one chiral centre, threo and

erythro isomers, methods of resolution, stereospecific and stereoselective synthesis, asymmetric synthesis, Cram's and Prelog's rules. Optical activity in the absence of chiral carbon-biphenyls, allenes and spiranes. Conformational analysis of cycloalkanes and decalins. Effect of conformation on reactivity. Acyclic & cyclic systems-Substituted cyclohexanes, cyclohexanones, cyclohexanols, Curtin-Hammet Principle. Stereochemistry of compounds containing nitrogen, sulphur and phosphorus. 12 hrs

**Geometrical Isomerism:** Cis-trans isomerism resulting from double bonds, monocyclic compounds & fused ring systems. E,Z-notations, determination of configuration of geometrical isomers, syn & anti isomers. 3 hrs

#### REFERENCES:

1. Organic Chemistry-P.Y. Bruice (Pearson Education Pvt. Ltd. New Delhi) 2002.
2. Stereochemistry, Conformation and Mechanism-P.S. Kalsi (Wiley Eastern, New Delhi) 1993.
3. Stereochemistry of Carbon Compounds-E.L. Eliel (Tata McGraw Hill, New. Delhi) 1994.
4. Advanced Organic Chemistry-Reactions, mechanisms & structure-J. March (Wiley, NY) 2000.
5. Organic Chemistry-Vol. -1, 2 &3-Mukherji, Singh and Kapoor. (Wiley Eastern) 1994.
6. A guide book of mechanisms in Organic Chemistry-P. Sykes (Orient- Longman) 1985.
7. Organic Chemistry-R.T. Morrison and R.N. Boyd (Prentice Hall, New Delhi) 1994.
8. Organic Chemistry 4<sup>th</sup>Edn.-S.H. Pine et al (McGraw-Hill, London) 1987.
9. Advanced Organic Chemistry- R.A. Carey and R.J. Sundberg (Plenum, New York) 1990.
10. Modern Concepts of Advanced Organic Chemistry-R.P. Narein (Vikas, Delhi) 1997.
11. A Text book of Organic Chemistry-Tewari, Vishnoi and Mehrotra (Vikas, New Delhi) 1998.
12. A Text book of Organic Chemistry-3<sup>rd</sup>Edn.-R.K. Bansal, (New Age, New Delhi) 1997.
13. Organic Chemistry-3<sup>rd</sup>Edn- F.A. Carey (Tata McGraw Hill, New Delhi) 1996.
14. Stereochemistry by K. Mislow.
15. Organic Chemistry-H. Pine (Hendrickson, Cram and Hammond, McGraw Hill, New York) 1987.
16. Organic Chemistry-I.L. Finar (ELBS Longmann, Vol. I) 1984.

## CH H 403: PHYSICAL CHEMISTRY

### COURSE OUTCOME:

- To understand the theoretical basis of catalysis, corrosion and various complex reactions which find relevance in biological processes and are of industrial importance.
- The students are introduced to the modern techniques developed for the practical applications of these concepts in different areas of science and technology.
- This course will enable the students to handle issues related to corrosion in the day to day life and in industrial reactors; enzyme mediated reactions in biochemistry, biotechnology and pharmaceutical chemistry etc.

### UNIT-I: Catalysis

[15hours]

**Catalysis:** Homogeneous Catalysis—equilibrium and steady state treatments, activation energies of catalysed reactions. Acid - base catalysis (general and specific), protolytic and prototropic mechanisms, catalytic activity and acid strength measurements. Kinetics of enzyme catalysed mechanisms – Michaelis – Menten mechanism. Effect of pH, temperature and inhibitors. 6hrs.

**Acidity functions:** Hammett acidity function, Zucker–Hammett hypothesis, and Bunnett hypothesis. 2hrs

**Surface Chemistry:** A review of adsorption isotherms, uni- and bi- molecular reactions. Multilayer adsorption: BET equation – application in surface area determination. Harkin – Jura equation and application. Semiconductor catalysis, n- & p- type. Mechanism of surface reactions. Langmuir – Hinshelwood and Langmuir Rideal mechanisms. 7hrs

### UNIT – II

[15 hours]

#### Chemical Kinetics:

**Composite reactions:** Rate equation for composite reaction mechanisms (simultaneous and consecutive reactions, steady state treatment, rate determining steps and microscopic reversibility), Chain reactions (hydrogen-halogen reactions with comparison). Auto catalytic reactions (Hydrogen-Oxygen reaction) and Oscillatory reactions. 6hrs.

**Reactions in solution:** Solvent effects on the reaction rates, Factors determining reaction rates in solution, reaction between ions (effect of dielectric constant and ionic strength), substitution and correlation effects (Hammett and Taft equations-linear free energy relations.) Ion-dipole and dipole-dipole reactions (Pre exp factors and influence of ionic strength) and diffusion controlled reactions. 4 hrs.

**Fast reactions-**Introduction, Study of fast reactions by-flow, relaxation, molecular beam, and spectroscopic and analytical methods. 3hrs.

**Theory of reaction rates-** Temperature dependence and the Arrhenius theory of reaction rates, collision theory of bimolecular reactions, its importance and limitations. Introduction to transition state theory. 2hrs.

### UNIT-III

[15hours]

**Electrochemistry of solutions:** Ionic atmosphere-introduction, derivation and its effect on the theory of conductivity. Walden's rule. Debye-Huckel limiting law (DHL), its modification and verification. Bjerrum theory of ion association, triple ion formation and its significance.

4hrs.

**Corrosion:** Introduction, Importance and principles, Forms of corrosion (Galvanic, Atmospheric, stress, microbial and soil). Techniques of Corrosion rate measurement (instrumental and non-instrumental). EMF series & galvanic series and their limitations. Thermodynamics (Pourbaix diagram). Concept of mixed potential theory and its importance in terms of Kinetics (Tafel and Evans diagram), effect of oxidizer and passivity of corrosion. Protection against corrosion (Design improvement, Anodic and cathodic protection, inhibitors, coating).

6 hrs

**Analytical Applications of Electrochemistry** -Principles and Applications of Polarography, Cyclic voltammetry, Coulometry, Amperometry and chrono systems.

5hrs

### REFERENCES

1. Chemical Kinetics, K. J. Laidler, Pearson Education, An and Sons (India) 3rd ed., 2008.
2. Fundamentals of Chemical Kinetics, M.R. Wright, Harwood Publishing, Chichesrer, 1999.
3. Kinetics & Mechanisms of Chemical Transformations, J Rajaram& J C Kuriacose, Macmillan, Delhi,42007.
4. Chemical &Electrochemical Energy Systems, R. Narayan & B. Viswanathan (University Press), 1998.
5. Industrial Electrochemistry, D. Peltcher & F. C. Walsh (Chapman & Hall)1990.
6. Principles and Applications of Electrochemistry–Crow (Chapman hall, New York) 2014
7. An Introduction to metallic corrosion and its prevention-Raj Narayan (Oxford-IBH, New Delhi), 1983.
8. Electrochemistry and Corrosion Science-Nebtor Ferez (Springer Pvt. Ltd.), Delhi, 2010.
9. Instrumental Methods of Chemical Analysis, Kudesia Sawhney, Pragati Prakasha (Meerut).

## CH S 404: SPECTROSCOPY AND ANALYTICAL TECHNIQUES

### COURSE OUTCOME:

- Students will learn the basic principles and applications of ESR Spectroscopy, NQR Spectroscopy,
- Students can be familiarising with Mossbauer Spectroscopy, Photoelectron spectroscopy, Atomic absorption Spectroscopy, Emission Spectroscopy, Molecular Luminescence Spectroscopy and Light Scattering methods.
- The students will also trained in the field of Ion Exchange Chromatography, Exclusion Chromatography and Thermal methods
- Overall students can solve the problems related to spectroscopy

### UNIT- I:

[12 Hours]

**Electron Spin Resonance Spectroscopy:** Basic principles, hyperfine couplings, the 'g' values, factors affecting 'g' values, isotropic and anisotropic hyperfine coupling constants, Zero Field splitting and Kramer's degeneracy. Measurement techniques and Applications to simple inorganic and organic free radicals and to inorganic complexes.

**NQR Spectroscopy:** Quadrupolar nuclei, electric field gradient, nuclear quadrupole coupling constants, energies of quadrupolar transitions, effect of magnetic field. Applications.

**Mossbauer Spectroscopy:** The Mossbauer effect, chemical isomer shifts, quadrupole interactions, measurement techniques and spectrum display, application to the study of  $\text{Fe}^{2+}$  and  $\text{Fe}^{3+}$  compounds,  $\text{Sn}^{2+}$  and  $\text{Sn}^{4+}$  compounds( nature of M-L bond, coordination number and structure), detection of oxidation states and inequivalent Mössbauer atoms.

**Photoelectron spectroscopy:** Basic principles, valence & core binding energies, shifts in energies due to chemical forces, Photoelectron spectra of simple molecules, Auger transitions, measurement techniques. Applications.

### UNIT-II

[12 Hours]

**Ion Exchange Chromatography:** Definitions, requirements for ion-exchange resin, synthesis and types of ion-exchange resins, Principles, basic features of ion-exchange reactions, resin properties, ion-exchange capacity, resin selectivity and factors affecting the selectivity, applications of IEC in preparative, purification and recovery process. Separation of lanthanides.

**Exclusion Chromatography:** Theory and principle of size exclusion chromatography, experimental techniques for gel-filtration chromatography (GFC) and gel-permeation chromatography (GPC), materials for packing-factors governing column efficiency, methodology and applications.

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

### UNIT – III:

[12 Hours]

**Atomic Absorption Spectrometry:** Principle, Theory, working of AAS instruments, analytical applications, interferences.

**Emission Spectroscopy:** Flame Emission Spectroscopy, plasma emission spectrometry, basic 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.

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

### REFERENCES:

1. A. Salahuddin Kunju and G. Krishnan: Group Theory and its Applications in Chemistry, PHI Learning, N. Delhi, 2010
2. Gurudeep Raj, Ajay Bhagi and Vinod Jain: Group Theory and Symmetry in Chemistry, 4th edn, Krishna Meetut, 2012.
3. U.C. Agarwala, H.L. Nigam, Sudha Agarwal and S.S. Kalra: Molecular Symmetry in Chemistry via Group Theory, Anne Books, N. Delhi, 2013.
4. G.D. Christian: Analytical Chemistry, (4th Ed.), (John Wiley), 1986.
5. R.A. Day and A.L. Underwood: Quantitative Analysis, 5<sup>th</sup> Ed. (Prentice Hall, India), 1998.
6. H.H. Wiliard, L.L. Merrit and J.J. Dean, Instrumental methods of analysis, (7<sup>th</sup> Ed.) 1988
7. B.K. Sharma, Instrumental Methods of Chemical Analysis (Goel publishing), 2000.
8. Skoog, Holler and Nieman: Principles of Instrumental Analysis, (Harcourt Afca), 2001



## CH S 405: ENVIRONMENTAL CHEMISTRY

### COURSE OUTCOME:

- This course enlighten the students about environmental pollutions like Air pollution, toxic chemicals in the environment,
- Hydrologic cycle, BOD, COD, radioactive waste management, sewage and industrial effluent treatment, water purification,
- Biochemical effects of Pesticides and heavy metals.
- Students learn effect of toxic chemicals in environment.

### UNIT-I

[12 Hrs]

Environmental segments, evolution of earth's atmosphere. Air pollution: Air pollutants, prevention and control, Green house gases and acid rain. Carbon monoxide, industrial sources and transportation sources. SO<sub>x</sub>- sources, ambient concentration, test methods, control techniques

- scrubbing, , limestone injection process. Ozone hole and CFC's. Photochemical smog and PAN. NO<sub>x</sub> - Sources, ambient concentration, test methods, thermodynamics and NO<sub>x</sub> control techniques. Particulates: Size distribution, particulate collection - settling chambers, centrifugal separators, wet scrubbers, electrostatic precipitators & fabric filters. Catalytic converters for mobile sources. Bhopal gas tragedy.

### UNIT-II

[12 Hrs]

Hydrologic cycle, sources, chemistry of sea water, criteria and standards of water quality-safe drinking water, maximum contamination levels of inorganic and organic chemicals, radiological contaminants, turbidity, microbial contaminants. Public health significance and measurement of colour, turbidity, total solids, acidity, alkalinity, hardness, chloride, residual chlorine, sulphate, fluoride, phosphate and different forms of nitrogen in natural and polluted water. Chemical sources of taste and odour, treatment for their removal, sampling and monitoring techniques. Determination and significance of DO, BOD, COD and TOC. Water purification for drinking and industrial purposes, disinfection techniques, demineralization, desalination processes and reverse osmosis.

### UNIT – III

[12hrs]

Toxic chemicals in the environment, impact of toxic chemicals on enzymes. Detergents-pollution aspects, eutrophication. Pesticides- pollution of surface water. Sewage and industrial effluent treatment, heavy metal pollution. Chemical speciation- biochemical effects of pesticides, insecticides, particulates, heavy metals (Hg, As, Pb, Se), carbon monoxide, nitrogen oxides, sulphur oxides, hydrocarbon, particulates, ozone, cyanide and PAN. Solid pollutants and its treatment and disposal. Radioactive waste management.

### REFERENCES:

1. A.K. De: Environmental Chemistry, (Wiley Eastern).
2. S.K. Banerji: Environmental Chemistry, (Prentice Hall India), 1993.
- 3 S.D. Faust and O.M. Aly: Chemistry of Water Treatment, (Butterworths),1983.
4. Sawyer and McCarty, Chemistry for Environmental Engineering (McGraw Hill) 1978
5. I. Williams, Environmental Chemistry, John Wiley, 2001
6. S.M. Khopkar, Environmental Pollution Analysis, (Wiley Eastern).

## CH S 406-Molecular Spectroscopy & Diffraction Techniques

### COURSE OUTCOME:

- Deals with the understanding of the spectroscopic techniques which are based on the interaction of the electromagnetic radiation in the microwave, infrared and X-ray region with the molecules.
- The techniques introduced here are major characterization techniques employed to understand the chemical composition of compounds and the physical characteristics.
- The course has multidisciplinary relevance as these techniques are used in various fields namely, chemistry, physics biology and materials science.
- Student will be able to learn instrument like x-ray, TEM, SEM and their applications

### UNIT-I

[12 hours]

**Introduction to spectroscopy**, intensity of spectral lines, Natural line width and broadening, Rotational, vibrational and electronic energy levels, selection rules.

**Microwave Spectroscopy**- The rotation and classification of molecules, rotation spectra of diatomic and polyatomic molecules. Rigid and non-rigid rotator models. Determination of bond length, isotope effect on rotation spectra. Stark effect, nuclear and electron spin interaction. Microwave Spectrometer.

**Vibration Spectroscopy**: Vibration spectra of diatomic molecules - linear harmonic oscillator, vibrational energies, zero point energy, force constants & bond strengths; anharmonicity of molecular vibrations- Morse PE diagram, selection rules, fundamental, overtones and hot bands. Vibrations of polyatomic molecules- normal modes of vibrations & nature of molecular vibrations (Ex-CO<sub>2</sub>& H<sub>2</sub>O).

### UNIT-II:

[12 hours]

Vibration-rotation spectra of diatomic and polyatomic molecules, selection rules, PQR branches. IR Spectrophotometer-Instrumentation

**Raman Spectroscopy**: Classical and quantum theories of Raman effect, concept of polarizability and polarizability ellipsoid. Rotational and vibrational Raman spectra, selection rules, Raman activity of vibrations, vibrational- rotational Raman spectra, selection rules, mutual exclusion principle, polarization of Raman lines. An introduction to Laser Raman Spectroscopy. Raman Spectrometer – instrumentation. Applications of IR and Raman spectroscopy in elucidation of molecular structure (Ex - H<sub>2</sub>O, N<sub>2</sub>O & CO<sub>2</sub> molecules).

### UNIT III

[12Hours]

**Diffraction Techniques**: Introduction, production of X-ray, Bragg's law, Laue equations, Ewald's diagram, X-Ray diffraction experiments – diffraction of X-rays by a crystalline powder (Debye-Scherrer and flat plate camera), powder diffract meter. Interpretation of power patterns (analytical technique). Single crystal technique - Laue and Rotation photographic methods. Moving Film method (Weissenberg method). Systematic absences. Crystalline X-ray diffractometer (4 angle), Intensities of diffracted X-rays and structural analysis, X-ray scattering atoms and molecules, Factors affecting X-ray intensities, introduction to Crystal structure analysis. 9hrs.

Electron Diffraction: Introduction, Theory of electron diffraction, Wierl equation and its significance (qualitatively), Elucidation of structure of simple gas molecules. Structure of

surfaces - (Low and high Energy Electron Diffraction, Transmission electron microscopy (TEM), SEM. Theory and applications of Neutron diffraction. Comparison between X-ray, electron and Neutron diffractions. 3hrs.

#### **REFERENCES:**

1. Fundamentals of Molecular Spectroscopy, Banwell & McCash (Tata McGraw Hill, New Delhi) 2007.
2. Spectroscopy, H. Kaur (Pragathi Prakashana, Meerut), 2012.
3. Spectroscopy, Donald L. Pavia (Cengage learning India Pvt. Ltd., Delhi), 2007.
4. Spectroscopy, B.K. Sharma (Goelprakashan, Meerut), 2013.
5. A Basic Course in Crystallography, JAK Tareen and TRN Kutty, University Press, Hyderabad (2001).
6. Essentials of Crystallography, M.A. Waheb, Narosa Publishing House, New Delhi (2009),
7. X-ray methods, Clive Whiston, (John Wiley & Sons, New York) 1987.



## CH P 407: INORGANIC CHEMISTRY PRACTICALS – I

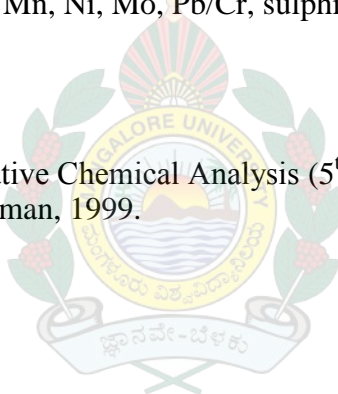
### COURSE OUTCOME:

- Students will have hands on experience on the analysis of Hematite Dolomite, Pyrolusite, Solder,
- Analysis of Halide Mixture, Colorimetric Determination, Gravimetric determinations and Statistical Analysis of Data.
- To understand Complex metric determination and hardness of water
- It enables the students to learn Statistical Analysis of Data.

1. Analysis of Hematite-insoluble residue by gravimetry and Iron by volumetry using  $Ce^{4+}$ .
2. Analysis of Dolomite - insoluble residue by gravimetry and Ca, Mg by complexometry.
3. Pyrolusite - Insoluble residue by gravimetry and Manganese content by oxalate method.
4. Analysis of solder - Pb and Sn by EDTA method.
5. Complex metric determination of Mn, Cu, Ni and Fe-Cr mixture
6. Hardness of water
7. Analysis of Halide Mixture - Iodide by  $KIO_3$  and total halide by gravimetrically.
8. Colorimetric Determination of Iron by thiocyanate and Cu by aqueous ammonia.
9. Gravimetric Determinations of Mn, Ni, Mo, Pb/Cr, sulphide, thiocyanate.
10. Statistical Analysis of Data.

### Reference:

1. Vogel's Text Book of Quantitative Chemical Analysis (5<sup>th</sup> Ed), G.H. Jeffrey, J. Bassette, J. Mendham and R.C. Denny, Longman, 1999.



## CH P 408: ORGANIC CHEMISTRY PRACTICALS – I

### COURSE OUTCOME:

- Enlighten the students to understand the method of organic preparation by utilizing various kinds of organic reactions,
- To understand isolation and purification of products.
- To understand oxidation reactions
- To learn substitution reaction.

### Single and two stage organic preparations

1. Electrophilic substitution reactions–Preparations of p-bromoaniline, p-nitroaniline, 2,4, 6-tribromophenol and picric acid.
2. Alkylations–Preparation of nerolin and N-methyl anthranilic acid.
3. Acetylations–Preparations of  $\alpha$ -D-glucose penta-acetate and 2-naphthyl acetate.
4. Reactions with ring formation–Preparations of 1, 2, 3, 4-tetrahydrocarbazole, 1-phenyl-3-methyl-5-pyrazolone and 7-hydroxy-4-methyl-coumarin.
5. Diazotisation reactions–Preparations of iodo, chloro and azo compounds.
6. Dehydration reactions–Preparations of cyclohexene and succinic anhydride
7. Condensation reactions–Condensations involving diethylmalonate and ethyl acetoacetate. Claisen-Schmidt, Aldol and Perkin condensation reactions.
8. Halogenation reactions-Preparation of n-butylbromide &  $\alpha$ ,  $\beta$ -dibromocinnamic acid.
9. Reduction reactions–Reductions of nitro compounds and carbonyl compounds.
10. Oxidation reactions-Preparation of p-nitrobenzoic acid, p-benzoquinone and adipic acid.

### REFERENCES:

1. Laboratory Manual in Organic Chemistry–R. K. Bansal (New Age, New Delhi)1990.
2. Experimental Organic Chemistry–Vol. I & II–P. R. Singh et al (TMH New Delhi)1981
3. Laboratory Manual in Organic Chemistry–Dey & Sitaraman (Allied, New Delhi) 1992.
4. Vogel's Text Book of Practical Organic Chemistry including Qualitative Organic Analysis - B. S. Furniss et al., (Longman - ELBS, London), 1989.
5. Manual of Organic Chemistry - Dey and Seetharaman.
6. A Text Book of Practical Organic Chemistry – A.I. Vogel, Vol.III.
8. Practical Organic Chemistry - Mann & Saunders.

## CH P 409: PHYSICAL CHEMISTRY PRACTICALS - I

(Any 12 experiments are to be carried out)

### COURSE OUTCOME:

- Experiments have been designed which make use of the concepts of electrochemistry, thermodynamics, solution chemistry and surface chemistry.
- Students get hands on experience in use of various instruments.
- It will be able to understand the theoretical concepts.
- To learn Specific and molar refractivity, viscosity, parachor etc.

1. (a) Determination of transport number of  $\text{Cd}^{2+}$  and  $\text{SO}_4^{2-}$  ions by EMF method.  
(b) Determination of thermodynamic parameters of a cell reaction by EMF method.
  2. Determination of pK values phosphoric acid by potentiometric/pH metric method
  3. Potentiometric titration of halides in mixtures ( $\text{Cl}^-$ ,  $\text{Br}^-$  and  $\text{I}^-$ ) with silver nitrate
  4. Verification of Nernst equation for  $\text{Ag}^+$ ,  $\text{Cu}^{2+}$  and  $\text{Zn}^{2+}$  species.
  5. Determination of Solubility product and the Instability constant by potentiometric method.
  6. Potentiometric determination of solubility of insoluble silver halide and the standard electrode potential using quinhydrone electrode.
  7. Conductometric titrations of displacement and precipitation reactions.
  8. Determination of equivalent conductance and dissociation constants of weak acid and base.
  9. Determination of solubility of lead iodide at different T & hence molar heat of solution
  11. Determination of hydrolysis constant of aniline hydrochloride.
  11. Determination of degree of hydrolysis of  $\text{CH}_3\text{CO}_2\text{Na}$  and  $\text{NH}_4\text{Cl}$  by conductivity method.
  12. Determination of Critical Micelle concentration by conductometric method.
  13. Determination of pH of buffer solutions with a pH meter & evaluation of  $\text{pK}_a$  of acids
  14. Verification of Walden's rule (relation between viscosity of a solution and the electrical Conductivity).
  15. Study of variation of viscosity of a liquid with temperature
  16. Determination of parachor value for  $\text{CH}_2$  group and some elements by Surface Tension method,
  17. Determination of the composition of a solution by S.T measurement
  18. Determination of the Critical Micelle Concentration by surface tension/spectrophotometric measurements.
  19. Determination of the composition of Zinc Ferrocyanide complex by Potentiometric titrations.
  20. Determination of Specific and molar refractivity of liquids and paracor value of a species by refractometric method.
- Any other relevant experiments of interest.

### REFERENCES:

1. Findlay's Practical Physical Chemistry- B. P. Levitt (Longman, London).
2. Experiments in Physical Chemistry– James and Prichard.
3. Experimental Physical Chemistry - Daniels et al.
4. Experimental Physical Chemistry-Das & Behera (Tata McGraw Hill, New Delhi)1983.
5. Advanced Practical Physical Chemistry–Yadav (1989).
6. Experiments in Physical Chemistry–J. C. Ghosh (Bharathi Bhavan)1974.
7. Practical Physical Chemistry-B Viswanathan & P.S Raghavan, (ViVa Books, New Delhi) 2005.

## 2<sup>nd</sup> Semester

### CH H 451: ADVANCED INORGANIC CHEMISTRY

#### COURSE OUTCOME:

- Students will study Symmetry and Group Theory,
- Chemistry of higher Boranes, Phosphazene polymers,
- Advances aspects of MOT theory, Trends of transition metals in periodic tables, Methods of reduction of oxide ores in this course

#### UNIT - I:

[15 Hours]

##### Symmetry and Group Theory

Definitions of group, subgroup, relation between orders of a finite group and its subgroup. Conjugacy relation and classes, symmetry elements and symmetry operations, Schonflies symbols, Matrix representations of symmetry operations, products of symmetry operations, some properties of matrices and vectors, classification of molecules into point groups.

Reducible and irreducible representations. The Great Orthogonality theorem (without proof), character tables. The direct product. Applications of group theory - Molecular vibrations, group theoretical selection rules for electronic transitions, for infra red and Raman spectra. Hybrid orbitals and Molecular orbitals, transformation properties of atomic orbitals.

#### UNIT – II:

[15 Hours]

Chemistry of higher boranes, classification, structure and M.O. description of bonding, framework electron counting, Wade's rules, chemistry of  $B_5H_9$ ,  $B_{10}H_{14}$  and  $B_nH_n^{2-}$  carboranes and metallocarboranes. Cyclophosphazenes, phosphazene polymers, S-N compounds. Coordination numbers 2-10 and their geometry, crystal field theory of coordination compounds, d-orbital splittings in octahedral, square planar and tetrahedral fields, spectrochemical series, and

Jahn-Teller effect. Structural evidences for ligand field splittings – hydration, ligation and lattice energies, site preference energies. MO theory of coordination compounds- MO energy level diagrams for octahedral and tetrahedral complexes.

#### UNIT - III:

[15 Hours]

Trends in oxidations states, stereochemistry and ionic sizes of metals, comparison of 3d, 4d and 5d series by taking Ti and Ni subgroups as examples. Lanthanides and actinides: electronic structure, oxidation states, extraction and separation of lanthanides, stereochemistry, spectral and magnetic properties of lanthanide and actinide complexes, lanthanide complexes as NMR shift reagents. Comparison with d-block ions.

Methods of reduction of oxide ores, Ellingham diagram, chemical and electrolytic reductions, reduction potentials, Latimer and Frost diagrams, effect of complexation on potential.

## REFERENCES:

1. J. E Huheey, E.A..Keiter, R.L. Keiter & O K Medhi: Inorganic Chemistry (4<sup>th</sup>edn.), Pearson, 2006.
2. Shriver, Atkins and Langford: Inorganic Chemistry (3<sup>rd</sup>edn.) OUP, 1999.
3. J.D. Lee: Concise Inorganic Chemistry, ( 5<sup>th</sup>edn.) Blackwell Science, 2000.
4. B.E. Douglas, D. McDaniel & A Alexander: Concepts & Models of Inorganic Chemistry, Wiley 2001
5. W.W. Porterfield: Inorganic chemistry – A Unified Approach, Elsevier, 2005.
- 6.N.N. Greenwood and A. Earnshaw, Chemistry of the Elements, First Edn (Pergamon Press)
7. Basallo & Johnson, Coordination Chemistry





## CH H 452: ADVANCED ORGANIC CHEMISTRY

### COURSE OUTCOME:

- Students will gain an understanding of all details of aliphatic/ aromatic electrophilic substitution reactions and aromatic nucleophilic substitution reactions.
- Students will learn about various free radical reactions and elimination reactions including pyrolytic eliminations.
- Students will gain an understanding of formation and hydrolysis of esters, Addition of carbon-carbon multiple bonds and addition to carbon-heteroatom multiple bonds.

### UNIT - I: [15 Hours]

**Aliphatic Electrophilic Substitution Reactions:** Bimolecular mechanisms- $S_{E1}$ ,  $S_{E2}$  and  $S_{Ei}$  mechanism. Electrophilic substitution reactions accompanied by double bond shifts. 3 hrs  
**Aromatic Electrophilic and Nucleophilic Substitution Reactions:** Mechanism of aromatic electrophilic substitution reactions-nitration, halogenation, sulphonation, Friedel-Crafts alkylation and acylation, orientation and reactivity, energy profile diagram. The ortho/para ratio, ipso attack, orientation in other ring systems. Mechanism of Vilsmeier-Haack reaction, Mannich reaction, Diazonium coupling, Pechmann reaction and Fries rearrangement. Mechanisms of aromatic nucleophilic substitution reactions-  $S_{N}Ar$ ,  $S_{N}1$  & aryne mechanism. Von-Richter rearrangement, Sommelet-Hauser rearrangement, Smiles rearrangement. 12 hrs

### UNIT- II: [15 Hours]

**Free Radical Reactions:** Types, mechanisms of free radical substitution reactions & neighbouring group assistance. Reactivity for the aliphatic and aromatic substances at a bridgehead. Reactivity of attacking radical. Effect of solvent on reactivity. Auto-oxidation, coupling of alkynes. Arylation of aromatic compounds by diazonium salts. Sandmeyer, Ullmann & Hunsdiecker reactions. 5 hrs

**Elimination Reactions:** Discussions of  $E1$ ,  $E2$  and  $E1cB$  mechanisms. Orientation during elimination reactions. Saytzeff and Hofmann rules. Reactivity-effects of substrate structures, attacking base, leaving group and solvent medium. 5 hrs

**Pyrolytic Eliminations:** Mechanisms of pyrolysis of esters of carboxylic acids. Chugaev reactions, Hofmann degradation, Cope elimination and xanthate pyrolysis. 5 hrs

### UNIT- III: [15 Hours]

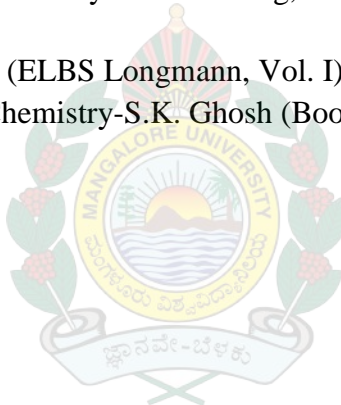
**Formation and Hydrolysis of Esters:** Plurality of mechanism. Mechanism of esterification reactions. Ester hydrolysis- $A_{AC}2$ ,  $B_{AC}2$ ,  $A_{AC}1$  &  $A_{AL}1$  mechanism. Transesterification. 4 hrs

**Addition to Carbon-Carbon Multiple Bonds:** Addition reactions involving electrophiles, nucleophiles and free radicals. Cyclic mechanisms. Orientation and stereochemistry. Addition of halogens, hydrogen halides, carboxylic acids and amines. Addition to cyclopropanes, hydroboration, Michael addition. Addition of oxygen across double bonds. 5hrs

**Addition to Carbon-Hetero Multiple Bonds:** Electrophilic, nucleophilic and free radical additions to C=O and C=N systems. Addition of Grignard reagents. Reformsky reaction, aldol condensation, Knoevenagel condensation, Perkin reaction and Wittig reactions. 6 hrs

#### REFERENCES:

1. Organic Reactions and Their Mechanisms- P.S. Kalsi (New Age, New Delhi),1996.
2. Advanced Organic Chemistry 4th Edn- J. March (Wiley, NY) 2000.
3. Organic Reaction Mechanisms- Bansal (Tata McGraw Hill, New Delhi) 1978.
4. Organic Chemistry-Vol.-I & II-Mukherji, Singh and Kapoor (Wiley Eastern, New Delhi) 1985.
5. Mechanism and Theory in Organic Chemistry-Lowry and Richardson Harper and Row, 1987.
6. Reaction Mechanisms in Organic Chemistry-Mukherji, Singh and Kapoor (McMillan) 1978.
7. Organic Chemistry-P.Y. Bruice (Pearson Education, New Delhi) 2002.
8. Organic Reaction Mechanism-R.K. Bansal (Wiley Eastern Limited, New Delhi) 1993.
9. A Guide Book to Mechanism in Organic Chemistry-Petersykes.
10. Advanced Organic Chemistry –Carey and Sundberg, Part A& B, 3rd edition (Plenum Press, New York) 1990.
11. Organic Chemistry-I.L. Finar (ELBS Longmann, Vol. I) 1984.
12. Advanced General Organic Chemistry-S.K. Ghosh (Book and Alleied (P) Ltd) 1998.



## CH H 453: ADVANCED PHYSICAL CHEMISTRY

### COURSE OUTCOME:

- It is an advanced level course which helps to understand the concepts of physics and their subsequent applications in the field of chemistry.
- The concepts of chemical thermodynamics helps in the design of processes in chemical industries.
- The concepts of statistical thermodynamics find relevance in understanding the nature of solids and metals in specific.
- It enables to understand chemical bonding, photochemistry and spectroscopy

### UNIT I:

[15hours]

#### Chemical Thermodynamics:

Entropy: Physical significance, entropy change in an ideal gas. Variation of entropy with Temperature, Pressure and Volume. Entropy change in reversible and irreversible processes. Thermodynamic equations of state.

Free energy, Maxwell's relations and significance. Helmholtz's and Gibbs free energies, Gibbs– Helmholtz equation and its applications.

Nernst heat theorem: Its consequences and applications. Third law of thermodynamics – statements, applications and Comparison with Nernst Heat theorem.

Chemical affinity and thermodynamic functions. Effect of temperature and pressure on chemical equilibrium- van't Hoff reaction isochore and isotherms.

Partial molar properties: Physical significance, determination of partial molar volume and enthalpy. Chemical potential: variation of chemical potential with temperature. Gibbs – Duhem equation.

Thermodynamic functions of mixing, Gibbs – Duhem – Margules equation.

Fugacity: Relationship between fugacity and pressure. Determination of fugacity- graphical method and Lewis Randall rule.

Activity and activity coefficient: Variation of activity and fugacity with temperature and pressure. Determination of activity by vapour pressure method.

### UNIT - II: Statistical and Irreversible thermodynamics

[15 hours]

**Statistical Thermodynamics:** Thermodynamic Probability, phase space, micro and macrostates, statistical weight factor, assembly, ensemble-significance, classification and comparison. Distribution laws – Boltzmann law, Maxwell-Boltzmann distribution law. Bose-Einstein and Fermi-Dirac statistics, Limit of applicability of various laws. Relationship between partition function and thermodynamic functions -Average energy, heat capacity, free energy, chemical potential. Introduction to Statistical mechanism of independent, independent and indistinguishable (non-localized) molecules or particles.

Partition function for molecular particles.

Thermodynamic quantities in terms of partition function of particles- Evaluation of Translational, vibrational, rotational, electronic and nuclear derivations of translational, rotational, vibrational and electronic partition functions. Law of equipartition principle. Partition function and equilibrium constant.

Statistical thermodynamic properties of solids (Heat capacity)-Introduction, thermal characteristics of crystalline solid, Einstein model, Debye modification. Nuclear statistics -

Introduction, symmetric and nuclear spin, ortho and para nuclear states. Applications of partition function to mono atomic gases, diatomic molecules, equilibrium constant. 9hrs.

**Irreversible Thermodynamics** – Introduction, Thermodynamics of irreversible processes, Entropy production-rate of entropy production. Phenomenological relations. The principle of microscopic reversibility, Onsager reciprocal relations – validity and applications (Electro kinetic, Thermoelectric phenomena). Irreversible thermodynamics of Non linear regime and biological systems. 6hrs

### UNIT III

Postulates of quantum Mechanics. Particle waves, its character and significance. Normalization and orthogonality of wave functions. Operators and their algebra, types and applications, operators for the dynamic variables of a system (position, linear momentum, angular momentum, Kinetic energy, potential energy and total energy) Eigen values and Eigen functions. Quantum numbers and their characteristics. Schrodinger wave equation – significance and derivation. Statistical interpretation of  $\psi$  7 hrs

Solution of SWE for simple systems-particle in a box (1D & 3D), particle in a ring, simple harmonic oscillator, rigid rotor, the H atom (solution of  $r, \theta, \Phi$  equations). Chemical Bonding in diatomics: Covalent bond-Valence bond and molecular orbital approaches with comparison.

Molecular orbital theory applied to homonuclear and heteronuclear diatomic molecules. Introduction to Huckel molecular orbital theory of conjugated systems and its applications. 8hrs

### REFERENCES:

1. Thermodynamics for Chemists- S Glasstone (East West press)
2. Physical Chemistry-P W Atkins.
3. Chemical Thermodynamics, Rajaram and Kuriokose (East-West) Pearson, Chennai, 2013.
4. Thermodynamics, 3<sup>rd</sup> Ed., R.C. Srivastava and Subit K Saha (Prentice-Hall of India, Delhi), 2007.
5. Statistical Thermodynamics, M. C. Gupta (New Age International, Delhi)2007.
6. Principles of Physical chemistry; B.R. Puri, L.R. Sharma and M.S. Pathania, Vishal Publishers (2014)
7. Atomic Structure and Chemical Bond, Manasa Chanda, Tata McGraw Hill Publishers (1991).
8. Quantum Chemistry, R.K. Prasad, New Age International (1991)
9. Advanced Physical Chemistry- Gurdeep R Chatwal (Goel Publishes, Meerut), 1992.
10. Introductory Quantum Chemistry – A.K. Chandra (Tata McGraw Hill) 1994.
11. Quantum Chemistry, A.B. Sannigrahi (Book and Allied Pvt. Ltd., Kolkatta), 2013.
12. Quantum Chemistry, Donald A.P (Viva Books, Delhi), 2013.

## CH S 454: ORGANIC SPECTROSCOPIC TECHNIQUES

### COURSE OUTCOME:

- Enable the students to understand the principle, theory, instrumentation and applications of UV-Visible, Electronic, NMR ( $^1\text{H}$ ,  $^{13}\text{C}$ ,  $^{19}\text{F}$ ,  $^{31}\text{P}$ ) and Mass spectroscopy.
- To solve the composite problems involving the applications of UV-Visible, IR, NMR ( $^1\text{H}$  &  $^{13}\text{C}$ ) and Mass spectroscopic techniques.
- To develop the ability to analyse the spectrum and arrive at the correct structure of compound.
- Overall students can get confidence in solving spectroscopic problems.

### UNIT-I: [12 hours]

**UV/Electronic Spectroscopy:** Basic principles, Chromophores, auxochromes, Instrumentation and application. Factors affecting the positions of UV bands. Electronic transitions and empirical correlations of predicting  $\lambda_{\text{max}}$  of organic compounds. Woodward-Fieser rules. UV absorption of aromatic compounds - effect of substituents and solvent effects. Empirical rules to calculate  $\lambda_{\text{max}}$ . Application of UV spectroscopy in the structural study of organic molecules. 5 hrs

**IR Spectroscopy:** Basic principles, Application of infrared spectroscopy in the structural study-identity by finger printing and identification of functional groups. Characteristic vibrational frequencies of common functional groups (alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols and amines). Study of vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters, amides, anhydrides and acids). Factors affecting band positions and intensities such as effect of hydrogen bonding, phase and solvent on vibrational frequencies, overtones, combination bands and Fermi resonance. 7 hr

### UNIT-II: Nuclear Magnetic Resonance Spectroscopy [12 hours]

Theory and principle, NMR spectrometer, FT NMR and its advantages. Solvents used, chemical shift and its measurements, factors affecting chemical shift. Integration of NMR signals, spin-spin coupling, coupling constant. Shielding and deshielding. Chemical shift assignment of major functional groups, Classification (ABX, AMX, ABC,  $A_2B_2$ ), spin decoupling, effects of chemical exchange, fluxional molecules, Hindered rotation through NMR spectrum, Karplus relationships (Karplus curve-variation of coupling constant with dihedral angle), double resonance techniques, NMR shift reagents, solvent effects and Nuclear Overhauser Effect. High resolution  $^1\text{H}$  NMR. Applications of NMR spectroscopy in structure elucidation of simple organic and inorganic molecules. Pulse techniques in NMR, two dimensional and solid state NMR. Use of NMR in Medical diagnostics. 10 hrs

**NMR of nuclei other than proton:**  $^{13}\text{C}$  chemical shift & factors affecting it. Decoupling-Noise decoupling & broad band decoupling. Off-resonance proton decoupling-some representative examples. Introduction to  $^{19}\text{F}$  &  $^{31}\text{P}$  NMR. 2 hrs

### UNIT-III: Mass Spectrometry [12 hours]

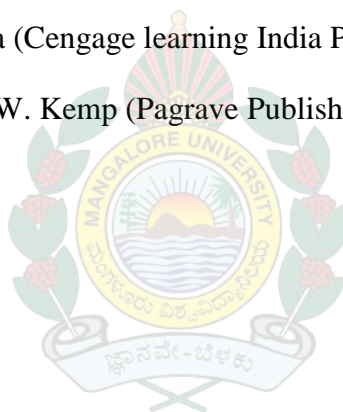
Basic principles, Instrumentation, interpretation of mass spectra, resolution, exact masses of nucleides, molecular ions, meta-stable ions and isotope ions. Fragmentation processes-representation of fragmentation, basic fragmentation types and rules. Factors influencing fragmentations and reaction pathways. McLafferty rearrangement. Fragmentations associated

with functional groups- alkanes, alkenes, cycloalkanes, aromatic hydrocarbons, halides, alcohols, phenols, ethers, acetals, ketals, aldehydes, ketones, quinines, carboxylic acids, esters, amides, acid chlorides, nitro compounds and amines. Ion analysis, ion abundance, retro Diels-Alder fragmentation. Nitrogen rule. High resolution mass spectroscopy. 9 hrs

Composite problems involving the applications of UV, IR,  $^1\text{H}$  and  $^{13}\text{C}$  NMR and mass spectroscopic techniques. Structural elucidation of organic molecules. 3 hrs

#### REFERENCES:

1. Spectrometric Identification of Organic Compounds - Silverstein, Bassler & Monnill (Wiley) 1981.
2. Applications of Absorption Spectroscopy of Organic Compounds-Dyer (Prentice Hall, NY) 1965.
3. Spectroscopy of Organic Compounds-3<sup>rd</sup> Ed.-P.S. Kalsi (New Age, New Delhi) 2000.
4. Analytical Chemistry-Open Learning: Mass spectrometry.
5. Spectroscopic Methods in Organic Chemistry - Williams and Fleming, TMH.
6. Spectroscopy, Donald L. Pavia (Cengage learning India Pvt. Ltd., Delhi), 2007.
7. Organic Spectroscopy-3<sup>rd</sup> ed.-W. Kemp (Pargrave Publishers, New York), 1991.



## CH S 455: ANALYTICAL AND GREEN CHEMISTRY

### COURSE OUTCOME:

- Enable the students to learn about cell structure and functions, lipids, lipoproteins.
- To understand the importance and functions of enzymes and coenzymes in biological systems.
- It helps in understanding metabolic pathways of cholesterol, bile acids, prostaglandins.
- Mechanism of reactions catalyzed by the above coenzymes.

### UNIT I:

**12 Hours**

**Cell Structure and Functions:** Structure of prokaryotic and eukaryotic cells, intracellular organelles and their functions, comparison of animal and plant cells. Overview of metabolic processes – catabolism and anabolism. ATP- the biological energy currency. Origin of life – unique properties of carbon, chemical evolution and rise of living systems.

**Lipids:** Fatty acids, essential fatty acids, structure and function of triacylglycerides, glycerophospholipids, sphingolipids, cholesterol, bile acids, prostaglandins.

**Lipoproteins:** composition and function, role in atherosclerosis, properties of lipid aggregates, micelles, bilayers, liposomes and their biological functions. Biological membranes- Fluid mosaic model of membrane structure. Lipid metabolism (-oxidation of fatty acids).

### UNIT II:

**12 Hours**

**Enzymes:** Introduction, Classification, Enzyme substrate complex formation models: Lock and Key model, Host-Guest and Induced- Fit model. Factors affecting enzyme activity (pH, temperature), enzyme inhibition (reversible and irreversible) and immobilised enzymes. Examples of some typical enzyme mechanisms for Triose phosphate isomerase,  $\alpha$ - Carboxy peptidase-A and Ribonuclease. Enzymatic synthesis of  $\alpha$ -amino acids and peptides. Transformations of lipases and esterases. Kinetic resolutions of carboxylic acids, esters and alcohols- Transesterification. Enzymatic synthesis of  $\alpha$ -amino acids and peptides. Transformations of lipases and esterases.

### Coenzymes

**12 Hours**

Introduction Co factors - co substrates - prosthetic groups. Classification-Vitamin derived coenzymes and metabolite coenzymes. Structure and biological functions of coenzyme A, thiamine pyrophosphate (TPP), pyridoxal phosphate (PLP), oxidized and reduced forms of nicotinamide adenosine dinucleotide / their phosphates (NAD, NADH, NADP<sup>+</sup>, NADPH), Flavin adenine nucleotide (FAD, FADH<sub>2</sub>), Flavin mononucleotide (FMN, FMNH<sub>2</sub>) and tetrahydrofolate. Adenosine triphosphate (ATP) and adenosine diphosphate (ADP). Mechanism of reactions catalyzed by the above coenzymes.

## REFERENCES:

1. Principles of Biochemistry – A L Lehninger, Worth Publishers.
2. Biochemistry – L Stryer, W H Freeman.
3. Biochemistry – J David Rawn and Neil Patters.
4. Biochemistry – Voet and Voet, John Wiley.
5. Outlines of Biochemistry – E E Conn and P K Stumpf. John Wiley.
6. Enzyme structure and mechanism - Fersht and Freeman
7. Outlines of Biochemistry - Conn and Stumpf
8. Principles of Biochemistry - Horton & others.
9. Bioorganic chemistry - A chemical approach to enzyme action - Herman Dugas and Christopher Penney.





## CH E 456: ENVIRONMENTAL, ELECTRO AND POLYMER CHEMISTRY

### COURSE OUTCOME:

- It is an elective course offered to students from disciplines other than chemistry.
- It aims at enhancing their general understanding of chemistry. Few important topics such as sources and detection of air pollution, batteries as power sources, devices of solar energy conversion,
- Polymers used in day to day life and for medical and technical applications will be taught.
- Awareness of plastic pollution and technique of plastic waste management

### UNIT-I:

[12 Hours]

Environmental segments, evolution of earth's atmosphere. Air pollution: Air pollutants, prevention and control, Green house gases and acid rain. Carbon monoxide, industrial sources and transportation sources.  $\text{SO}_x$ - sources, ambient concentration, test methods, control techniques - scrubbing, limestone injection process. Ozone hole and CFC's. Photochemical smog and PAN.  $\text{NO}_x$  - Sources, ambient concentration, test methods, thermodynamics and  $\text{NO}_x$  control techniques. Particulates: Size distribution, particulate collection - settling chambers, centrifugal separators, wet scrubbers, electrostatic precipitators & fabric filters. Catalytic converters for mobile sources. Bhopal gas tragedy.

### UNIT-II

[12 hrs]

Corrosion: Introduction, consequence, type, prevention, & measurement. Conventional sources of energy, limitations, Importance of storage, Battery-Electrodes, Cell, battery Brief account of primary, secondary, lithium battery and fuel cells. Semiconductor electrodes and Solar energy system. 7 hrs

Introduction to bioelectrochemistry, electrochemical communication in biological organisms.

Theory and applications of Electroplating and electroless plating. 7hrs

Reaction Kinetics-Theory and applications of different types of reactions- Oscillatory, chain reaction, branched chain reaction. . Energy of activation and thermodynamic parameters, Collision theory of reaction rates limitations and basics of transition state theory. 5 hrs

### UNIT- III

[12 hrs]

Polymers: Introduction-Basic concepts and classification of polymers, Molecular weight and its distribution, Chemistry of polymerization- Step, chain, Coordination, Copolymerization. Polymerization techniques- bulk, solution, suspension, emulsion, poly-condensation, solid and gas phase polymerization. Chemical and geometrical structure of polymer molecules, Structure property relationship-Physical, Thermal and mechanical properties 6hrs  
Synthesis, properties, structural features and applications of some important commercial polymers (PE, PP,PS, PVC, PMMA, PET, Nylon-6,Nylon-6,6) , Engineering polymers (Kevlar, Nomex, ABS, PC, Teflon). Applications of polymers in separations: reverse osmosis, ultra and nano-filtration. Applications in electronics- conducting polymers and electronic shielding, Applications of polymers in medicine.  
Management of plastics in environment- recycling, incineration and biodegradation. 6hrs

## REFERENCES:

1. A.K. De: Environmental Chemistry, (Wiley Eastern).
2. S.K. Banerji : Environmental Chemistry, ( Prentice Hall India), 1993.
3. Sawyer and McCarty, Chemistry for Environmental Engineering (McGraw Hill) 1978.
4. An Introduction to metallic corrosion and its prevention-Raj Narayan (Oxford-IBH, New Delhi), 1983.
5. Chemical & Electrochemical Energy Systems, R. Narayan & B. Viswanathan (University Press), 1998.
6. Industrial Electrochemistry, D. Peltcher & F. C. Walsh (Chapman & Hall)1990.
7. F.W. Billmeyer, Text book of Polymer science, 3rd Edn, A Wiley- Interscience Publication, New York, 2005
- 8.. V.R. Gowariker, Polymer Science, New Age International (P) Ltd., New Delhi, 2012
9. R.W. Dyson, Specialty Polymers, Chapman and Hall, New York, 1987
10. J.R. Fried, Polymer Science and Technology, Prentice Hall of India Pvt. Ltd., New Delhi, 1999
11. P. Ghosh, Polymer Science and Technology, Tata - McGraw Hill, New Delhi, 1995



## CH P 457: INORGANIC CHEMISTRY PRACTICALS-II

### COURSE OUTCOME:

- The students will have hands on experience in the qualitative analysis of mixtures of Inorganic Salts containing 3 cations in which 1 less common metal ion and 2 anions.
- Students will learn the systematic methods of separation techniques.
- Apart from inorganic radicals they also learn the separation organic radicals.

Qualitative Analysis of mixtures of Inorganic Salts containing 3 cations and 2 anions (1 less common metal ions like Tl, W, Mo, V, Zr, Th, U, Ce, Ti and Li to be included among anions organic acid radicals, phosphate, borate and fluoride separation included).

### REFERENCES:

1. Vogel's Text Book of Quantitative Chemical Analysis (5<sup>th</sup> Ed), G. H. Jeffrey, J. Bassette, J. Mendham and R. C. Denny, Longman, 1999
2. Vogel's Qualitative Inorganic Analysis (7<sup>th</sup> Ed), G. Svehla, Longman (2001).

## CH P 458: ORGANIC CHEMISTRY PRACTICALS-II

### COURSE OUTCOME:

- Student will gain the in-depth knowledge and skill in organic separations, purifications, qualitative analyses.
- Separation of binary mixtures of organic compounds containing both mono and bifunctional groups
- Students will learn preparation of suitable derivatives.

Separation and systematic qualitative analysis of binary mixtures of organic compounds containing both mono and bifunctional groups and preparation of suitable derivatives.

### REFERENCES:

1. Practical Organic Chemistry-F .G. Mann and B. C. Saunders (ELBS, England), 2001.
2. Practical Organic Chemistry - A. I. Vogel (Longman-ELBS, England), 1971.
3. Experimental Organic Chemistry–Vol.I & II Singh et al(TMh, New Delhi)1981.
4. Semimicro Qualitative Organic Analysis–Cheronis et al Wiley-Eastern, New Delhi) 1964.
5. Vogel's Text Book of Practical Organic Chemistry Including Qualitative Organic Analysis- B. S. Furniss *et al* (Longman-ELBS, England), 1978.
6. Manual of Organic Chemistry - Dey and Seetharaman.
7. Modern Experimental Organic Chemistry-John H. Miller and E.F. Neugil.

## CH P 459: PHYSICAL CHEMISTRY PRACTICALS- II

(At least 12 experiments are to be carried out)

### COURSE OUTCOME:

- In continuation with the practical course introduced in the first semester, this course provides opportunity to students to test the concepts learnt in the basic physical chemistry course CH H 403.
- Experiments have been designed on thermodynamics, kinetics, surface and interface chemistry. With the training gained.
- Students will be able to handle issues related to metallurgical processes, waste water treatment, energy efficient processes, action of soaps and detergents etc.

1. Determination of cryoscopic constants of solvents and molecular weight of non volatile substances by thermal method.
2. Determination of degree of dissociation, Vant Hoff factor and molecular weight of an electrolyte by cryoscopy method using copper calorimeter/Dewar flask..
3. Heat of solution of a sparingly soluble compound in water by solubility method.
4. Phase diagram of two component systems by thermal analysis.
5. Phase diagram of three component system (a) 3 liquids with single binodal curve, and b) two liquids and one solid
6. Kinetics of acid catalyzed hydrolysis of methyl acetate and determination of (a) order and rate constant and (b) Energy of activation.
7. Determination of a) Energy of activation & b) rate constant for the First and second order kinetics of reaction between potassium per sulphate and potassium iodide.
8. Kinetics of sodium formate – iodine reaction.
9. Determination of the latent heat of evaporation of carbon tetrachloride.
10. Preparation of colloidal solutions.
11. Verification of F & L adsorption isotherms for acetic acid on activated charcoal.
12. To study the adsorption of iodine on charcoal from alcoholic solution.
13. To study the effects of gelatin solution on the precipitation values.
14. Comparison of detergent action of detergents and determination of interfacial tension.
15. Thermodynamic prediction and measurement of the solubility of naphthalene in benzene. Study of association of benzoic acid in benzene/toluene. Any other relevant experiments of interest.

## REFERENCES:-

1. Practical Physical Chemistry- B Viswanathan & P.S Raghavan, (ViVa Books, Delhi) 2005.
2. Findlay's Practical Physical Chemistry- B. P. Levitt (Longman, London).
3. Experiments in Physical Chemistry– James and Prichard.
4. Experimental Physical Chemistry - Daniels et al.
4. Experimental Physical Chemistry-Das &Behera (Tata McGraw Hill, New Delhi)1983.
5. Advanced Practical Physical Chemistry–Yadav (1989).
6. Experiments in Physical Chemistry–J. C. Ghosh (Bharathi Bhavan)1974.



## 3<sup>rd</sup> SEMESTER

### CH H 501: COORDINATION CHEMISTRY

#### COURSE OUTCOME:

- The students will learn spectral properties of complexes, interpretation of spectra
- Photochemistry of metal complexes, Magnetic behavior of metal complexes,
- Spectral applications of coordination compounds,
- Reactions mechanisms in Transition metal complexes, Electron transfer reactions.

#### UNIT- I: [15 Hours]

Spectral properties of complexes: Term symbols for  $d^n$  ions, spectroscopic ground states, selection rules, nature of spectral bands- band shapes, band intensities, band widths, spin-orbit coupling, vibrational structures.

Orgel diagrams, Tanabe-Sugano diagrams, interpretation of spectra of octahedral, distorted octahedral, tetrahedral and square planar complexes, Determination of  $\nu$  from spectra. Charge transfer bands – origin, types, and characteristics. Photochemistry of metal complexes- photosubstitution and photoredox reactions, ligand photoredox reactions, photoreactions and solar energy conversion.

#### UNIT- II: [15 Hours]

Type of magnetic behaviour, orbital contribution, spin orbit coupling, spin cross-over systems. Measurement of magnetic susceptibility – Gouy and Faraday methods, diamagnetic corrections, ferro- and antiferromagnetic coupling, super paramagnetism. High and low spin equilibria. Magnetic properties of lanthanides and actinides. Infrared spectra of metal complexes, Group frequency concept. Changes in ligand vibrations on coordination- metal ligand vibrations. Spectral applications of coordination compounds - IR spectra of metal carbonyls - ESR spectra-application to copper complexes, Mossbauer spectra- application to iron complexes. NMR spectra - Application to diamagnetic complexes.

#### UNIT- III: [15 Hours]

Reaction Mechanisms in Transition Metal Complexes: Energy profile of a reaction, inert and labile complexes, kinetics of octahedral substitution and mechanistic aspects. Acid hydrolysis, factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism and evidences in its favor. Anation reactions, reactions without M-L bond cleavage. Substitution reactions in square planar complexes, trans effect, mechanisms of substitution. Substitution reactions in tetrahedral complexes. Isomerization and racemization reactions of coordination compounds. Electron transfer reactions- inner sphere and outer sphere reactions, complimentary and non-complimentary reactions.

#### REFERENCES:

1. D.N. Satyanarayana: Electronic absorption Spectroscopy and Related Techniques, OUP, 2001.
2. F. Basolo and R.G. Pearson: Inorganic Reaction Mechanisms, Wiley Eastern, 1979.
3. W.W. Porterfield: Inorganic chemistry – A Unified Approach, Elsevier, 2005.
4. R.L. Dutta and A Syamal : Elements of Magnetochemistry, Affiliated east-West, 1993.
5. J.E Huheey, R.L. Keiter and A.L. Keiter: Inorganic Chemistry(4<sup>th</sup>edn), Addison Wesley, 2000.

## CH H 502: ORGANIC REACTION MECHANISM AND HETEROCYCLIC CHEMISTRY

### COURSE OUTCOME:

- Students will gain the in-depth knowledge about ten organic name reactions, their mechanisms and synthetic uses with multiple examples.
- Students will learn about the mechanism and synthetic utility of various kinds of thirteen molecular rearrangement reactions with diverse examples.
- Students will gain knowledge on principles of photochemistry and diverse types of photochemical reactions of organic molecules with multiple examples, concepts of pericyclic reactions, diverse types of electrocyclic, cycloaddition and sigmatropic reactions with multiple examples.
- Students will understand the systematic nomenclature of various types of heterocyclic compounds with multiple examples.
- Students will get the sound knowledge on the structure, synthesis and reactions of various three, four, five, six and seven membered simple and fused heterocyclic compounds.

### UNIT I:

[15 Hours]

**Organic Name reactions:** Reactions, Mechanisms and synthetic uses of Darzen's glycidic ester condensation, Cannizzaro reaction, Benzoin condensation, Claisen-Schmidt condensation, Stork Enamine reactions, Sharpless asymmetric epoxidation, Suzuki coupling, Heck reaction, Woodward and Prevost Hydroxylation and Mitsunobu reaction.

**Molecular rearrangements:** Mechanism and synthetic utility of Wagner-Meerwein, Dienone-Phenol, Pinacol-Pinacolone, Demjanov, Benzil-Benzilic acid, Fries, Wolff, Favorskii, Benzidine, Baker-Venkatraman, Beckmann, Bayer-Villiger and Amadori rearrangement.

### UNIT II:

[15 Hours]

**Organic Photochemistry:** Bonding and antibonding orbital, Chemistry of excited states of organic molecules, Jablonski diagram and quantum yield, Photo dissociation, Photo reduction, Photochemical isomerisation, Norrish Type-I and Type-II reactions, Barton reaction and Photo Fries rearrangement, Paterno-Buchi reaction, Yang cyclization, photo oxidation and photo catalysis.

**Pericyclic Reactions:** Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl systems. Woodward-Hoffmann correlation diagram and FMO approach.

**Electrocyclic Reactions:** Introduction, Con-rotatory & dis-rotatory Process,  $4n$  &  $4n+2$  systems. **Cycloaddition reaction:** Suprafacial and Antarafacial addition,  $2+2$  and  $4+2$  systems. 1,3-Dipolarcycloaddition reactions.

**Sigmatropic reactions:** Suprafacial and Antarafacial shift of H, [1,3] & [1,5] -sigmatropic shifts.

**UNIT- III:****[15 Hours]**

**Heterocyclic Chemistry:** Nomenclature of Heterocycles, Hantzsch-Widman system formonocyclic, fused and bridged heterocycles. Structure, synthesis and reactions of three membered heterocycles (aziridines, episulfides, diaziridines, oxazirines), four membered heterocycles (azetidines and thietanes), five membered heterocycles (furan, pyrrole, thiophene, oxazoles, imidazoles, thiazoles), six membered heterocycles (pyridine, Pyrimidine,  $\alpha$ - and  $\gamma$ -Pyrones), seven membered heterocycles (Azepines, Oxepines, Thiepinines) and fused heterocycles (Indoles, benzofurans, Quinolines, Isoquinolines, Coumarins, Purines).

**REFERENCES**

1. O.L. Chapman, Organic Photochemistry. Vol I & II. Marcel Decker.
2. Francis A Carey and R. J. Sundberg, Advanced Organic Chemistry-Part A & (Plenum).
3. Mukherji Singh and Kapoor, Organic Chemistry, Vol 1-3, (Wiley Eastern, New Delhi)
4. Synthetic Organic Chemistry- G.R. Chatwal (Himalaya, Bombay), 1994.
5. Organic Reaction Mechanisms, V.K. Ahluwalia & R.K. Parashar (Narosa) 2006
6. Organic Chemistry, Vol I-II, I.L. Finar, (Longmann ELBS, London), 1973.
7. Advanced Organic Chemistry- Reaction Mechanisms, Reinhard Bruckner (Academic) 2005.
8. Pericyclic reactions, S.M Mukherji (The McMillan Bangalore), 1979.
9. Organic Reactions and their mechanisms- P.S. Kalsi (New Age, New Delhi), 1996.
10. An Introduction to the Chemistry of Heterocyclic Compounds-Acheson (Wiley-Eastern) 1987.
11. Heterocyclic Chemistry-J. Joule & G. Smith (Van-Nostrand) 1978.
12. Heterocyclic Chemistry, 3<sup>rd</sup> Edition-Raj K. Bansal (New Age International) 2005.
13. Organic Chemistry-P.Y. Bruice (Pearson Education, New Delhi) 2002.
14. Comprehensive Heterocyclic Chemistry Vol-I-VI Ed. Katritzky & Rees (Pergamon), 1984.



## CH H 503: SOLID STATE CHEMISTRY

### COURSE OUTCOME:

- It is an interdisciplinary course falling at the boundary of physics and chemistry.
- It is aimed at understanding the properties of solids and their possible applications in materials science as superconductors, semiconductors, liquid crystal materials and as magnetic materials.
- Importance has been given to the methods of preparation of solids, understanding the structure-property relationships and their possible applications.
- Importance has also been given to the advanced topics of nanomaterials.

### UNIT-I:[15hours]

**Surface morphology:** Structure of solid surfaces and adsorbed layers. Mechanism of surface reactions. 3hrs.

**Crystal Defects and Non-Stoichiometry:** Imperfections and defects in crystals. Vacancy, Schottky and Frenkel defects. Thermodynamics of Schottky and Frenkel defect formation, colour centres, non-stoichiometry and defects—Structures of  $UO_2$ ,  $FeO$  and  $TiO_2$ .

4hrs.

**Solid State Reactions:** General Principles, Wagner's theory. Order- disorder transitions in solids- Bragg- William's theory Mechanism of diffusion, Kirkendall effect. 3 hrs

**Preparative Methods:** Ceramic, sol-gel, precursor and chemical vapour deposition (CVD) methods. Nucleation & crystal growth techniques-pulling, zoning, flame fusion & skull melting. Basic methods of preparation of thin films. 5 hrs

### UNIT-II:[15hours]

**Electronic Properties and Band Theory:** Free electron theory to band theory of solids, electrical conductivity, Hall effect. Metals, Insulators and Semiconductors. Intrinsic and extrinsic semiconductors, hopping semiconductors. Metal – semiconductor and p-n junctions. 6 hrs

**Magnetic properties:** Classification of magnetic materials—dia, para, ferro, ferri, antiferro & antiferri magnetic types Langevin diamagnetism. Selected magnetic materials such as spinels & garnets. 4hrs **Ionic Conductors:** Types of ionic conductors, mechanism of ionic conduction, diffusion superionic conductors; phase transitions and mechanism of conduction in superionic conductors, examples-□-alumina, AgI, halide and oxide ion conductors 5 hrs

### UNIT - III:

[15 Hours]

**Superconductivity:** Meissner effects; Types I and II superconductors, Features of superconductors, isotope effect, high  $T_c$  materials. Basics of low temperature superconductivity. 5hrs.

**Liquid Crystals:** Mesomorphic behaviour, thermotropic liquid crystals, positional order, bond orientational order, nematic and smecticmeso phases; smectic – nematic transition and clearing temperature- homeotropic, planar and schlieren textures, twisted nematics chiral nematics, molecular arrangements in smectic A & C phases. Optical properties of liquid crystals 5hrs

**Nanomaterials:** Introduction—importance and characterization of nanomaterials—stability of nanoparticles In solutions – synthesis of metal nanomaterials: Physical methods (Laser Ablation, Evaporation, sputtering and solvated metal dispersion) chemical methods (Thermolysis, Sonochemical approach, reduction of metal ions by hydrogen and methanol) 5hrs.

## REFERENCES:

1. D. K. Chakrabarty, Solid state chemistry (New Age) 1996.
2. H.V. Keer, Principles of the solid state (Wiley Eastern) 1993.
3. A.R. West, Solid state chemistry and its applications (Wiley) 1984.
4. L. Smart and E. Moore, Solid State Chemistry –An Introduction (Chapman &Hall) 1992.
5. L. Azaroff, An Introduction to Solids (Mc Graw Hill).
6. V. Raghavan, Material science and Engineering (3<sup>rd</sup> Ed), (Prentice Hall India) 1993.
7. Thermotropic Liquid Crystals, Ed. G.W. Gray, Wiley.
8. S. Chandrasekhar, Liquid Crystals, Cambridge University Press (2<sup>nd</sup>ed), 1994.
9. Chemical Kinetics, K. J. Laidler, Pearson Education, Anand Sons (India) 3<sup>rd</sup> edition (2008)
10. Physical Chemistry at surfaces, 6<sup>th</sup> ed., A.W Adamson and A P Gast, John Wiley, Canada, 1997.
11. C.P. Poole and F.K. Owens Introduction to Nanotechnology, (2004).
12. T. Pradeep, Nano: The Essential, Tata McGraw Hill Publishing Company Ltd., New Delhi, (2008).



## CH S 504: Medicinal and Natural Products Chemistry

### COURSE OUTCOME:

- Students will gain an understanding on the classification and nomenclature of drugs, modern theories of drug action and drug design.
- Students will be able to know classification, synthesis and mode of action of antipyretic analgesic drugs, general anaesthetics, local anaesthetics, cardiovascular drugs, antineoplastic agents and antiviral drugs with suitable examples.
- Students will get a good understanding of isolation, classification,
- Methods of structure elucidation and synthesis of various types of alkaloids, terpenoids and steroids with suitable examples.

### UNIT- I:

[12 Hours]

**Drugs:** Introduction, Classification and nomenclature of drugs. Theories of drug action-Occupancy theory, Induced fit theory and Perturbation theory. Analogues and Prodrugs, Factors governing drug design. Rational approach to drug design, Variation method of drug designing, Physico-Chemical factors, stereochemistry and biological activities. Factors governing the ability of drugs.

**Antipyretic Analgesics:** Classification, synthesis & mode of action of Phenacetin, Aspirin, Cinchophen, Phenazone and Mefenamic acid.

**General Anesthetics:** Introduction and classification, synthesis & mode of action of methoxyfluorane, Thiopental sodium and Fentanyl citrate.

**Local anesthetics:** Introduction and classification, synthesis & mode of action of benzocaine,  $\alpha$ -Eucaine, Lignocaine hydrochloride and Dibucaine hydrochloride.

### UNIT- II:

[12 hours]

**Cardiovascular drugs:** Introduction & classification, Synthesis & mode of action of Hydralazine, Methyldopa, Diazoxide, Procainamide, Propranolol, Prenylamine.

**Antimalarials:** Introduction and classification, Synthesis & mode of action of Chloroquinephosphate, Pamaquine and pyrimethanin.

**Antineoplastic agents:** Introduction and classification, Synthesis & mode of action of Mechlorethamine hydrochloride, Busulfantriethylenemelamine, Methotrexate and Flurouracil.

**Antiviral drugs:** Introduction, classification, Synthesis & mechanism of action of Methisazone, Idoxuridine and Amantidine hydrochloride.

### UNIT- III:

[12 Hours]

**Alkaloids:** Isolation, classification and general methods of structure elucidation. Structure and synthesis of Papaverine, Adrenaline and Reserpine.

**Terpenoids:** Introduction, classification, isoprene rule and methods of structure determination.

Structure and synthesis of Geraniol, Menthol,  $\alpha$ -Pinene, Camphor and Zingiberene.

**Steroids:** Introduction, Blanc's rule, Chemistry of Cholesterol, Oestrone, Progesterone and Androsterone.

**REFERENCES:**

1. Medicinal Chemistry- Ashutosh Kar (New Age.), 2005,
2. Medicinal Chemistry- G. R. Chatwal (Himalaya) 2002.
3. Principles of Drug Action- II Ed. A. Goldstein Lewis Arnold & Suner M. Kalman (Wiley Int. Ed.)
4. Natural Products Chemistry, Vol-I & II- G.R. Chatwal (Himalaya), 1990.
5. Organic Chemistry, Vol I & II, I.L. Finar (Longmann ELBS, London), 1973.
6. Chemistry of Natural Products – Vol-I & II – O. P. Agarwal (Goel Gorakhpur), 1985.
7. Chemistry of Natural Products: A Unified Approach-N R Krishnaswamy (University Press) 1999



## CH S 505: BIOORGANIC CHEMISTRY

### COURSE OUTCOME:

Students will be able to:

- Understand the configuration and conformation of monosaccharide's, chemistry of important derivatives of monosaccharide's, structure, synthesis, industrial and biological applications of disaccharides, general methods of determination of polysaccharide structures, photosynthesis, fermentation, structure and industrial applications of polysaccharides.
- Explain the peptide bond formation, synthetic protocol for peptides, solution and solid phase peptide synthesis, Methods of peptide structure determination, different types protein structures, non-steroidal hormones, nucleosides, nucleotides,
- Synthesis of nucleosides, nucleotides and polynucleotides, structure and functions of nucleic acids.
- Learn the classification, nomenclature, sources, deficiency diseases, biological functions and chemistry of Vitamin A1, B3, B5, C and K1.
- Know the classification and chemistry of antibiotics like Penicillin V, Streptomycin, chloramphenicol and tetracyclins

### UNIT I

[12 Hours]

**Carbohydrates** Configuration and conformation of (D & L) monosaccharide's, Hudson's rule, Mutarotation, Anomeric effect, Epimerization. Chemistry of important derivatives of monosaccharides: Glycosides (ethers, esters, acetals, ketals), deoxysugars, aminosugars, Structure of disaccharides-maltose, cellobiose and sucrose, Industrial & biological applications. General methods of structural degradation of polysaccharides- methylation & partial hydrolysis, Smith degradation and alkaline degradation techniques. Structures of cellulose, chitin, starch and glycogen. Industrial applications of cellulose & starch. Photosynthesis and Fermentation.

### UNIT II

[12 Hours]

**Peptides & Proteins:** Peptide bond formation and synthesis of polypeptides, Amino and carboxy protecting groups in peptide synthesis, Solid phase peptide synthesis-Merrifield method, Peptide structure determination-Sequence and End group analysis (N-Terminal and C-Terminal), Secondary, Tertiary and Quaternary structure of proteins.

**Nucleic acids:** Nucleosides and Nucleotides, Chemical synthesis of nucleosides and nucleotides. Poly nucleotides- Structure and functions of DNA and RNA.

**Non steroidal hormones:** Study of the Oxytocin, Vasopressin and synthetic analogs, General study of ACTH, Growth hormones, Somatotropin and Insulin.

### UNIT III

[12 Hours]

**Vitamins:** Classification and Nomenclature. Source, deficiency diseases and biological functions of Vitamins. Study of Vitamin A1, Vitamin B3, Vitamin B5, Vitamin C and Vitamin K1.

**Antibiotics:** Introduction, Classification, Chemistry of Penicillin V, Streptomycin, Chloramphenicol and Tetracyclin.

**REFERENCES:**

1. Organic Chemistry-P.Y. Bruice (Pearson Education Pvt.Ltd., New Delhi),2002.
2. Organic Chemistry 4<sup>th</sup>Edn.–S.H. Pine et al (McGraw-Hill, London) 1987.
3. Advanced Organic Chemistry- R.A. Carey and R.J. Sundberg (Plenum, New York)1990.
4. Organic Chemistry, Vol I & II, I.L. Finar (Longmann ELBS, London), 1973.
5. Natural Products Chemistry, Vol-I & II- G.R. Chatwal (Himalaya), 1990.
6. Chemistry of Natural Products: A Unified Approach-N R Krishnaswamy (University Press) 1999.
7. Chemistry of Natural Products-Sujata V. Bhat, B.A. Nagasampagi, Meenakshi Sivakumar (Springer-Narosa) 2005.



## CHE 506: ANALYTICAL & GREEN CHEMISTRY

### COURSE OUTCOME:

Enable the students:

- To understand the basic principles and theory of UV-Visible, Electronic, Infra Red, Nuclear Magnetic Resonance and Mass Spectroscopy.
- To study the utility of these techniques in structure elucidation of simple organic molecules.
- To know about water cycle, water sources, water quality, significant measurements of water parameters and treatment of water for drinking and industrial purposes.
- To learn about principles and use of green chemistry in laboratory synthesis.
- To understand the basic principles and utility of sonochemistry and Microwave induced organic synthesis.

### UNIT- I:

[12 Hours]

**UV/Electronic Spectroscopy:** Basic principles, Beer-Lambert law, types of absorption bands, Factors affecting the positions of UV bands. Theoretical prediction of  $\lambda_{\text{max}}$  for polyenes, -unsaturated aldehydes, ketones (Woodward-Fieser rules) and substituted benzenes.

**IR Spectroscopy:** Basic principles, Application of infrared spectroscopy in the structural study-identity by finger printing and identification of functional groups. Characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols and amines). Study of vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters, amides and acids). Factors affecting band positions and intensities

**Nuclear Magnetic Resonance Spectroscopy:** Basic principles, Solvents used, chemical shift and its measurements, factors affecting chemical shift. Integration of NMR signals, spin-spin coupling, coupling constant. Shielding and deshielding. High resolution  $^1\text{H}$  NMR. Applications of NMR spectroscopy in structure elucidation of simple organic molecules.

**Mass Spectrometry:** Basic principles, molecular ions, meta-stable ions and isotope ions. Fragmentation processes, McLafferty rearrangement. retro Diels-Alder fragmentations. Nitrogen rule.

### UNIT- II:

[12 Hours]

Hydrologic cycle, sources, chemistry of sea water, criteria and standards of water quality-safe drinking water, maximum contamination levels of inorganic and organic chemicals, radiological contaminants, turbidity, microbial contaminants. Public health significance and measurement of colour, turbidity, total solids, acidity, alkalinity, hardness, chloride, residual chlorine, sulphate, fluoride, phosphate and different forms of nitrogen in natural and polluted water. Chemical sources of taste and odour, treatment for their removal, sampling and monitoring techniques. Determination and significance of DO, BOD, COD and TOC. Water purification for drinking and industrial purposes, disinfection techniques, demineralization, desalination processes and reverse osmosis. Treatment of liquid radioactive wastes

**UNIT- III:****[12 Hours]**

**Green Chemistry:** Definition and principles, planning a green synthesis in a chemical laboratory, Green preparation-Aqueous phase reactions, solid state (solventless) reactions, photochemical reactions, Phase transfer catalyst catalysed reactions (Quaternary ammonium salts & Crown ethers), enzymatic transformations & reactions in ionic liquids.

**Sonochemistry:** Introduction, instrumentation, the phenomenon of cavitation, Sonochemical esterification, substitution, addition, oxidation, reduction and coupling reactions.

**Microwave induced organic synthesis:** Introduction, reaction vessel and reaction medium, concept, specific effect, atom efficiency, % atom utilisation, advantages and limitations, alkylation of active methylene compounds, N-alkylation, condensation of active methylene compounds with aldehydes, Diels-Alder reaction, Leuckardt reductive amination of ketones, ortho ester Claisen rearrangement.

**REFERENCES:**

1. Organic Spectroscopy-3<sup>rd</sup> Ed.-W. Kemp (Pargrave Publishers, New York), 1991.
2. Spectrometric Identification of Organic Compounds - Silverstein, Bassler & Monnill (Wiley)1981.
3. Applications of Absorption Spectroscopy of Organic Compounds-Dyer (Prentice Hall, NY) 1965.
4. Spectroscopy of Organic Compounds-3<sup>rd</sup> Ed.-P.S. Kalsi (New Age, New Delhi) 2000.
5. Spectroscopic Methods in Organic Chemistry - Williams and Fleming, TMH.
6. A.K. De: Environmental Chemistry, (Wiley Eastern).
7. S.K.Banerji : Environmental Chemistry, ( Prentice Hall India), 1993.
8. S.D. Faust and O.M. Aly: Chemistry of Water Treatment, (Butterworths),1983.
9. Sawyer and McCarty, Chemistry for Environmental Engineering (McGraw Hill) 1978
10. I. Williams, Environmental Chemistry, John Wiley, 2001
11. S.M. Khopkar, Environmental Pollution Analysis, (Wiley Eastern).
12. Organic Synthesis-Special Techniques, V.K. Ahluwalia& R. Aggarwal, Narosa, 2001.
13. Green Chemistry-Environment friendly alternatives- R. Sanghi & M.M. Srivatsava, Narosa, 2003.
14. Green Chemistry-Environment benign reactions- V.K. Ahluwalia, Ane Books India, 2006.



## CH P 507: INORGANIC CHEMISTRY PRACTICALS – III

### COURSE OUTCOME:

- The students will have hands on experience in the Analysis of Brass, Cu-Ni alloy, Stainless Steel,
- Type Metal and quantitative analysis of the constituents & mixtures containing the following radicals  $Fe^{+}$  Ni,  $Fe^{+}$  Ca,  $Cr^{+}$  Fe.
- This course also train the students in Separation and determination of  $Mg^{2+}/Zn^{2+}$ ,  $Zn^{2+}/Cd^{2+}$  by Ion-Exchange Chromatography in Part A and in Part B
- Determination of COD, Phosphorus, DO, Nitrate, Alkalinity of Water.

### A. Any five of the following experiments are to be carried out:

1. Analysis of brass-Cugravimetrically using  $\square$ -Benzoinoxime& Zinc complexometrically.
2. Analysis Cu-Ni alloy.
3. Analysis of Stainless Steel – Insoluble residue by gravimetry, Ni gravimetrically using DMG, Fe volumetrically using Ce(IV) & Cr(III) volumetrically by persulphate oxidation.
4. Analysis of Type metal–Sn gravimetrically, Pbelectrogravimetrically and Sb titrimetrically using  $KBrO_3$
5. Quantitative analysis of the constituents & mixtures containing the following radicals
  - i.  $Fe(II) + Ni(II)$  - Fe gravimetrically as  $Fe_2O_3$  and Ni using EDTA.
  - b.  $Fe(III) + Ca(II)$  - Fe gravimetrically as  $Fe_2O_3$  and Ca using EDTA.
  - c.  $Cr(III) + Fe(III)$  – Using EDTA by Kinetic masking method.
6. Analysis of chalcopyrites, magnetite and ilmenite.
7. Ion-exchange chromatography: Separation and determination of  $Mg^{2+}/Zn^{2+}$ ,  $Zn^{2+}/Cd^{2+}$  &  $Cl^-/Br^-$ .

### B. Any five of the following experiments are to be carried out:

8. Determination of COD of a water sample
9. Determination of Phosphorus.
10. Determination of dissolved oxygen (DO) by Winkler's method
11. Determination of nitrate & nitrite in water samples and sea water.
12. Analysis of heavy metals in waste water, sea water (Pb, Hg etc. By spectrophotometry)
13. Determination of available K in soil,
14. Nephelometric determination of sulphate/phosphate.
15. Determination of alkalinity of water samples
16. Determination of fluoride in drinking water by spectrophotometry and ion selective electrode
17. Determination of phosphates in detergents
18. Spectrophotometric determination of sulphur and phosphorus present in soil.

### REFERENCES:

1. A.I. Vogel: A Text book of Quantitative Inorganic Analysis, (ELBS), 1978.
2. APHA, AWWA and WPCF: Standard Method for the Examination of water and Waste Water (Washington DC),1989,
3. I. M. Kolthof and E.P. Sandell: Quantitative Chemical Analysis.McMillan,1980
4. I. Williams, Environmental Chemistry, Wiley, 2001
5. Lobinski and Marczenko, Comprehensive Analytical Chemistry, Vol.30, Elsevier,1996.

## CH P 508: ORGANIC CHEMISTRY PRACTICALS – III

### COURSE OUTCOME:

- Enable the students to understand and learn the principle of quantitative estimation of different types of organic molecules,
- Methods of organic preparations using multistep synthetic protocol,
- Isolation and purification of intermediate and final products,
- Use of computers in the study of conformation and geometry of some simple organic molecules.

**Quantitative Determination:** of sugars, amino acids, phenols, amines by various methods. Determinations of acid & ester and acid & amide in the given mixtures.

**Multi Step Organic Synthesis:** Synthesis of Ethyl resorcinol from Resorcinol,  $\epsilon$ -Caprolactam from cyclohexanone, p-Aminobenzoic acid from p-Nitrotoluidine, s-Tribromobenzene from aniline, Benzanilide from Benzophenone, Benzylic acid from Benzoin, 2,5-Dihydroxy acetophenone from Hydroquinone, 2,4-Dinitrophenylhydrazine from Chlorobenzene, m-Nitrobenzoic acid from Benzoic acid, 2,4-Dinitrophenol from Chlorobenzene, o-Aminobenzoic acid from Phthalic anhydride.

**Separation Techniques:** Separation of components from mixture of organic compounds by fractional crystallization, fractional distillation, adsorption, Paper and TLC. Their purification and characterization.

**Applications of computers** in the study of conformation and geometry of some simple organic molecules.

### REFERENCES:

1. Elementary Practical Organic Chemistry-Vol. III quantitative Organic Analysis- A.I. Vogel
2. Experimental Organic Chemistry- Vol. I &II- P.R. Singh, Tata McGraw-Hill, 1981.
3. Practical Organic Chemistry- IV Ed- Dey &.Sitaraman (Allied)
4. Laboratory Experiments in Organic Chemistry-Adam, Johnson &Wicon (McMillan, London), 1979.
5. Experimental Organic Chemistry- H.D. Durst &G.E. Goke (McGraw-Hill)1980.
6. Computers and their applications to Chemistry, Ramesh Kumari (Narosa).
7. Short Manual to the Chemical Drawing Program-Chem Draw®- Stefan Bienz (Cambridge Soft)

## CH P 509: PHYSICAL CHEMISTRY PRACTICALS – III

### COURSE OUTCOME:

- This practical course give training to students on important electrochemical techniques namely,
- Conductometry, potentiometry, voltametry and polarography.
- In addition, they are introduced to nuclear and radiation chemistry experiments.
- This course enhances the skill of students in quantitative analysis

### A. Electrochemistry:

#### a. Conductometry (At least three experiments to be carried out)

1. Titration of a mixture of acetic acid, monochloro and trichloacetic acids with NaOH.
2. Determination of concentrations/amounts of sulphuric acid, acetic acid and copper sulphate by conductometric titration with sodium hydroxide.
3. Measurements of the conductance of a weak acid, (a) HOAC and of the strong electrolytes NaOAc, HCl and NaCl and (b) HCOOH and of the strong electrolytes HCOONa, HCl and NaCl) and to calculate the ionization constant of the acid.
4. Titration of mixture of strong acid and weak acid with weak base (HCl + HAC against NH<sub>4</sub>OH).
5. Determination of pK<sub>a</sub> of a given weak acid by pH measurements at various dilutions.
6. Conductometric titration of the mixture of (a) HCl and NH<sub>4</sub>Cl and (b) HCl and acetic acid.
7. Determination of activity coefficient of Zinc ions in 0.002M ZnSO<sub>4</sub>.
8. Conductometric determination of Critical Micelle Concentration.

#### B. Potentiometry (At least three experiments are to be carried out)

1. Composition of Zinc Ferrocyanide Complex by potentiometric Titration.
2. Potentiometric titration of (a) Non aqueous system and (b) mixture of strong (HCl) and weak (HAC) acid with NaOH / NH<sub>4</sub>OH and find the strength of the acids in mixture.
3. Determination of decomposition potential of an aqueous electrolytic solution.
4. Determination of the potential of an electrochemical cell and mean ionic activity coefficient.
5. Determination of acidic and basic dissociation constants and isoelectric point an amino acid pH metrically..
6. pH titration of (a) HCl versus NaOH, (b) HOAC versus NaOH and (c) lead nitrate versus potassium chromate, and Titration of mixture of bases (Na<sub>2</sub>CO<sub>3</sub>& NaHCO<sub>3</sub>) with standard HCl..
7. Determination of pK<sub>a</sub> values of functional groups in amino acids using a pH meter.
8. Determination of Hammett constants of o-, m-, p- amino/nitro benzoic acid by pH measurements.
9. Verification of Tafel equation of hydrogen evolution reaction.
10. Study of rate of corrosion and inhibition efficiency of an inhibitor on mild steel/Al/Cu by weight loss method i) at different time intervals and ii) at different temperatures(to evaluate thermodynamic parameters)

### **C. Radiochemistry Experiments** (At least Three experiments to be carried out)

1. Study of (a) Characteristic plateau, (b) Geometry effects and Statistics of G.M counter
2. Determination of (a) Dead time by single source & double source method. (b)  $E_{max}$  of  $\alpha$  - source (c) Back scattering of  $\alpha$  and (d)  $\alpha$  energy emitted by C-14.
3. Verification of the inverse square law.
4. Determination of half life of radionuclides.
4. Determination of Linear and mass attenuation coefficient.
5. Preparation of Fricke and Ceric sulphate dosimeters & calculation of G-value & dose rate.
6. Study of isotope dilution analysis; 8. Radiochemical Determination of I-131 in sea water.
7. Determination of  $\beta$ -particle range and, axmum energy (by half thickness method).

### **C. Voltammetry & Polarography** (Any Three experiments are to be carried out)

1. Determination of the half-wave potential of Cd (II), Cu(II)& Zn(II) ions in 0.1M solutions.
2. Determination of metal ions individually and in mixtures,
3. Determination of the formula and the stability constant of a lead oxalate.
4. Study of the polarogram of supporting electrolyte with and without dissolved oxygen,
5. Determination of Huckel  $\log K$  value of aromatic hydrocarbon reduction at dropping mercury electrode.
6. Amperometric titrations.
7. Coulometric titration
8. Percentage purity of copper sulphate by electrogravimetric method.

### **REFERENCES:**

1. Findlay's Practical Physical Chemistry- B. P. Levitt (Longman, London).
2. Experiments in Physical Chemistry-James and Prichard.
3. Experimental Physical Chemistry - Daniels et al.
4. Experimental Physical Chemistry-Das & Behera (Tata McGraw Hill, New Delhi)1983.
5. Advanced Practical Physical Chemistry-Yadav (1989).
6. Experiments in Physical Chemistry-J. C. Ghosh (Bharathi Bhavan)1974.
7. Nucleonix systems Pvt. Ltd, Hyderabad.

## 4<sup>th</sup> SEMESTER

### CH H 551 BIOINORGANIC CHEMISTRY

#### COURSE OUTCOME:

- In this course, students will learn metal and non metal ions in biological systems,
- Biological nitrogen fixation, Photocatalysis,
- Transport and storage of dioxygen, Metal storage and Transport, Metalloproteins as enzymes,
- Therapeutic uses of metals, Metal complexes as drugs, Treatment of toxicity due to inorganics.

#### UNIT -I:

[15 Hours]

Metal and non metal ions in biological systems-essential and trace metals, ion transport across membranes, active transport of ions across biological membranes, ionophores.

Biological nitrogen fixation, Molybdenum nitrogenase Model compounds, in vitro fixation of nitrogen through dinitrogen complex. Metal complexes in transmission of energy-chlorophylls. photosystems I and II in cleavage of water, model systems.

#### UNIT-II:

[15Hours]

Transport and storage of dioxygen- heme proteins, oxygen uptake, functions of haemoglobin, myoglobin, hemerythrin and hemocyanins, synthetic oxygen carriers.

Metal storage and transport – ferritin, transferrin and ceruloplasmin. Electron transfer proteins-cytochromes, iron-sulphur proteins. Metalloproteins as enzymes – carboxy peptidase, carbonic anhydrase, alcohol dehydrogenase, catalases, peroxidases, cytochrome P 450, superoxide dismutase, copper oxidases, vitamin B12 coenzyme.

#### UNIT – III

[15 HOURS]

Therapeutic uses of Metals - Metals in medicine: Metals and human biochemistry, general requirements. Disease due to metal deficiency and treatment: Iron, zinc, copper, sodium, potassium, magnesium, calcium and selenium.

Metal complexes as drugs and therapeutic agents: Antibacterial agents, antiviral agents, metal complexes in cancer therapy, metal complexes for the treatment of rheumatoid arthritis, vanadium in diabetes, metal complexes as radio diagnostic agents.

Treatment of toxicity due to inorganics: General aspects of mechanism of metal ion toxicity, (i) Mechanism of antidote complex with poison, rendering it inert: arsenic, lead, mercury, iron, copper (ii) Antidote accelerated metabolic conversion of poison to non-toxic product: cyanide and carbon monoxide

#### REFERENCES

1. M.N. Hughes: Inorganic Chemistry of Biological Processes, (2<sup>nd</sup> edn.) Wiley, 1988.
2. I. Bertini. H.B. Gray, S.J. Lippard and J.S. Valentine: Bioinorganic Chemistry, Viva Books, 1998.
3. J.E Huheey, R.L. Keiter and A.L. Keiter: Inorganic Chemistry (4<sup>th</sup> edn), Addison Wesley, 2000.
4. K. Hussain Reddy, Bioinorganic Chemistry - New Age International Ltd. (2003).
5. R.W. Hay, Bioinorganic Chemistry - Ellis Horwood Ltd., (1984)
6. Asim K Das, Bioinorganic chemistry, Books & Allied (P) Ltd.

## CH H 552: ORGANIC SYNTHETIC METHODS

### COURSE OUTCOME:

Enable the students:

- To acquire knowledge on the various reagents employed for oxidation and reduction of various kinds of organic molecules.
- To understand the various methods of halogenations of carbonyl compounds, benzylic and allylic halogenations.
- To understand the synthetic design with diverse chemical reactions, planning of organic synthesis and functionality.
- To learn the principles and technologies used in disconnection approach, the utility of protecting group strategy in organic synthesis and retrosynthetic analysis.

### UNIT-I:

[15Hours]

**Reduction Reactions:** Catalytic hydrogenation-Introduction, catalysts and solvents, mechanisms and stereochemistry of catalytic hydrogenations. Hydrogenolysis and homogeneous catalytic hydrogenation.

**Metal hydride reduction:** Reduction with  $\text{LiAlH}_4$  and  $\text{NaBH}_4$ , Stereo chemistry of reduction, Reduction with diborane and related reactions.

**Dissolving Metal Reductions:** Mechanisms of reduction of carbonyl compounds, bimolecular reductions of esters, Birch reduction, Wolf-Kishner reduction and reduction with diimide. **Oxidation reactions:** Mechanism of oxidation reaction with chromium and manganese salts, Osmium tetroxide, peracids, periodic acid and Lead tetra acetate.

**Halogenation:** Halogenation of carbonyl compounds. Benzylic and Allylic halogenations.

### UNIT- II:

[15 Hours]

**Synthetic Design:** Carbon skeleton frame work, Classification of carbon-carbon single bond and double bond forming reaction and their use in carbon skeleton ring formation. Ring forming and ring cleaving reactions, use of Thorpe condensation, Carbene insertion reaction, Friedel-Crafts reaction, 1,3-dipolar addition and Ene reaction in ring formation, Oxidative cleavage of rings and Retro Diel's-Alder reactions.

**Planning of Organic Synthesis:** Selection of starting materials and key intermediates during the synthesis. Synthesis of Cubane and Iswarane. Use of Robinson annulation, Dieckmann cyclisation, Arndt-Eistert synthesis, Diel's- Alder reaction in organic synthesis.

**Functionality:** Synthesis of 6- and 7- methoxytetralones, biotin and penicillin-V with special reference to the introduction of functional groups. Stereo chemical consideration and stereo selectivity during organic synthesis.

### UNIT- III:

[15 Hours]

General introduction to disconnection approach. Basic principles and technologies used in disconnection approach. Synthons and synthetic equivalents. Interconversion of functional groups. One group C-X and two group C-X disconnections. Use of C-C one group and C-C two group disconnections in the synthesis of 1,2; 1,3; 1,4; 1,5 and 1,6-difunctionalised compounds. **Protecting groups:** Principle of protection of hydroxyl, amino, carboxylic and carbonyl groups.

**Retrosynthetic analysis:** Analysis of alcohols, carbonyl compounds cyclic and acyclic alkanes, benzocaine, p-methoxyacetophenone, acetonecyanohydrin, 2-methyl-6-methoxy-indole-3-acetic acid, 6-methylquinoline & 1-phenyl-4-p-methoxyphenyl-1,3-butadiene. Illustrative synthesis of Limonene, Danishefsky's pentalenolactone, Benziodarone,

Nitrofurazone, Warfarin, Juvabione, Longifolene, Prelog-Djerassi lactone and Taxol. Solid phase synthesis of oligonucleotides.

**REFERENCES:**

1. Modern Organic Reactions- H.O. House.
2. Organic Synthesis- R. E. Ireland (Prentice Hall India), 1969.
3. Art in Organic Synthesis- Anand, Bindra & Ranganath-(Wiley New Delhi), 1970.
4. Organic Synthesis a Disconnection Approach- Stuart Warren
5. Advanced Organic Chemistry-IV-Ed. Part A & B-F.J. Carrey & R.J. Sundberg (Kluwer) 2001.
6. Modern Methods of Organic Synthesis-N. Carruthers (Cambridge University), 1996.
7. Selected Organic Synthesis-Ian Fleming (John Wiley & Sons) 1973.



## CH H 553: ELECTROCHEMISTRY AND REACTION DYNAMICS

### COURSE OUTCOME:

- It is an advanced course on two different topics, electrochemical processes and theoretical aspects of chemical kinetics. The first part deals with concept and applications of electrocatalysis and processes taking place at the electrode and the solution interface.
- This course content trains students on alternate methods of synthesis using electrochemical concepts.
- Introduces the student to theoretical basis of understanding the rates of complex reactions,
- Arriving at the mechanism of various inorganic and organic reactions and knowledge of advanced techniques with the use of lasers in characterizing intermediates complex chemical reactions.

### UNIT-I:

[15 hours]

**Electrocatalysis** -Introduction. Electrocatalysis in reactions involving adsorbed species, concept and process of electrogrowth on electrodes. deposition to crystallization, mechanism of electrogrowth. Special features of electrocatalysis. Hydrogen evolution and reactions. Electronation of oxygen and their mechanisms. 6hrs.

**Photocatalysis:** History of photocatalysis, principles and developments in photoelectrochemistry. Semiconductor-electrolyte solution interface. Effect of light at semiconductor interface. Capacity of space charge - Mott-Schottky plot. Photo cells-PEC cells and Phtogalvanic cells, surface effects in photoelectrochemistry. 5hrs

**Ionic liquids** - Introduction, characteristics of ionic liquids, models of simple ionic liquids, mixtures of simple ionic liquids. Hole model for liquid electrolytes. Transport phenomena in liquid electrolytes. Electronic conductance of alkali metals dissolved in alkali halides. 4hrs.

### UNIT – II

[15 hours]

**Electrode Processes:** Charge transfer across the interface and its implications. Basic electrodic reactions: Butler - Volmer equation. Current potential laws at charged interface. Quantum aspects of charge transfer reactions. Concepts of over voltage, Theory of hydrogen and oxygen overvoltage. Mechanism of cathodic and anodic reactions, Dependence of current density on overvoltage: Tafel equation. Applications of electrode processes-(voltammetry, electrosynthesis, electrocatalysis, source of energy) 6 hrs.

**The Electrified Interface:** Electrification of an interfaces, experimental techniques used in studying interface (Low energy electron diffraction, X-ray photoelectron spectroscopy). The potential difference across Electrified interface. The accumulation and depletion of substances at an interface. Thermodynamics of electrified interface. Brief introduction to the structure of electrified interfaces(models) . 6hrs.

**Kinetics of Composite Reactions:** Inorganic reaction mechanism (decomposition of  $N_2O_5$ , and phosgene). Organic reaction mechanism- decomposition of acetaldehyde. Goldfinger-Letort-Niclause rules, combustion of hydrocarbon. 3hrs

### UNIT – II

[15 hours]

**Reaction Dynamics:** A Review of Chemical Kinetics, and activation parameters. Statistical treatment of rates – Transition state theory and its applications to reactions in solution. Concept of tunneling. Conventional transition state theory (CTST) - equilibrium hypothesis, Applications of CTST to reaction between atoms, derivation of rate expression, thermodynamic formulation of conventional transition – state theory, limitations of CTST.



Extension of TST.

7hrs.

**Potential energy surfaces** – Features & construction of them. Theoretical calculation of  $E_a$ . Features of potential energy surfaces (attractive and repulsive surfaces for exothermic reaction). A brief account on concept of stripping and rebound mechanisms. State-to-state kinetics and spectroscopy of transient species.

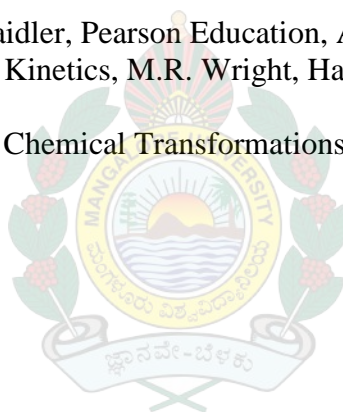
4hrs

Dynamics of unimolecular reactions - Lindemann, Hinshelwood, RRK & RRKM theories.

4 hrs.

#### REFERENCES:

1. Modern Electrochemistry, 2<sup>nd</sup> Ed. Vol.1, 2A &2B, J O M Bockris and A K N Reddy, (Plenum, New York) 1998.
2. Chemical and Electrochemical Energy Systems, Narayan & Viswanathan (Univ. Press, Hyderabad) 1998.
3. Fundamentals of Electrochemistry, Fulkner and A. J. Bard, Wiley India, 2006.
4. Ions in solution-Basic principles of chemical interactions, J. Burgeess (Chichester) 1999.
5. Electrochemistry-Principles, Methods and Applications, Brett and Brett, Oxford Science 1993.
6. Chemical Kinetics, K. J. Laidler, Pearson Education, Anand Sons (India) 3<sup>rd</sup> ed., 2008.
7. Fundamentals of Chemical Kinetics, M.R. Wright, Harwood Publishing, Chichesrer, 1999.
8. Kinetics & Mechanisms of Chemical Transformations, J Rajaram & J C Kuriacose, Macmillan, Delhi, 2007.



## CH S 554: ORGANOMETALLIC CHEMISTRY

### COURSE OUTCOME:

- The students will learn Historical development of Organometallic compounds, Classification,
- Nomenclature, Transition metal to carbon multiple bonded compounds, Transition metal-carbon pi complexes,
- Catalysis by organometallic compounds, Homogeneous catalysis by organometallics, Hydrocarbonylation of olefins,
- Ziegler-Natta catalyst and Water Gas Shift reactions in this course.

### UNIT- I:

[12 Hours]

Historical development- classification and nomenclature, bond energies and stability. 16- and 18-electron rules. Transition metal alkyls and aryls- types, routes of synthesis, stability and decomposition pathways. Nucleophilic and electrophilic cleavage of metal-carbon sigma bonded compounds. Alkane activation.

Transition metal to carbon multiple-bonded compounds- carbenes, carbynes, synthesis, nature of bond, agostic interactions, structural characteristics and reactivity. Transition metal hydrides– synthetic routes, properties, structure and reactivity, synthetic applications.

### UNIT-II:

[12 hours]

Transition metal-carbon pi complexes: Preparative methods, nature of bonding, structural features of olefinic, acetylenic, allylic, butadiene, cyclobutadiene,  $\eta^5$ - cyclopentadienyl,  $\eta^6$ - benzene and other arenes, cycloheptatriene and cyclooctatetraene complexes. Important reactions relating to nucleophilic and electrophilic attack on ligands. Fluxional isomerism in olefin, allyl, dienyl and cyclopentadienyl complexes. Carbene complexes and metallacycles, arene complexes. Isolobal concept.

### UNIT- III:

[12 hours]

Catalysis by organometallic compounds: oxidative addition, insertion, deinsertion and reductive elimination reactions.

Homogeneous catalysis by organometallics- hydrogenation, hydrosilation, hydrocyanation and isomerization of olefins, immobilisation of homogeneous hydrogenation catalysts, Hydrocarbonylation of olefins (oxo reaction–cobalt and rhodium oxo catalysts), Wacker process. Carbonylation of alcohols- Monsanto acetic acid process. Polymerization of olefins and acetylenes: Ziegler-Natta catalyst systems. Fischer – Tropsch reaction , Water Gas Shift reactions.

### REFERENCES:

1. J.P. Collman, L.S. hegedus, J.R. Norton and R.G. Finke: Principles and Applications of Organotransition Metal Chemistry, University Science Books, 1987.
2. R.C. Mehrotra and A. Singh: Organometallic Chemistry, New Age International, 1999.
3. R.H. Crabtree: Organometallic Chemistry of Transition Metals, Wiley, 1999.
4. F.A. Cotton and G. Wilkinson: Advanced Inorganic Chemistry, Wiley, 1991.
5. Organometallic Chemistry, G. S. Sodhi, Ane books Pvt Ltd Edition 2009.

## CH S 555: POLYMER CHEMISTRY

### COURSE OUTCOME:

- This is an introductory course on highly useful materials, namely the polymers. The course content is of interdisciplinary interest.
- It deals with types, techniques of preparation and characterization of plastics, rubber and fibre materials.
- The applications of these materials in daily life, engineering and biomedical field have been emphasized.
- The students are exposed to the problems of polymer waste management and the strategies developed to minimize plastic pollution.

### UNIT- I: [12 Hours]

**Terminology and basic concepts:** Monomers, Functionality, repeat UNITS, degree of polymerization. General structure and naming of polymers. **Classification** based on various considerations-source, preparation methods, thermal behavior, chain structure etc.

**Types** –Homopolymers and copolymers; Linear, branched and network polymers.

**Techniques of polymerization:** Techniques of preparation of addition and condensation polymers.

**Kinetics of polymerization:** Kinetics of addition and condensation polymerization. Kinetics of copolymerization.

### UNIT- II: [12 Hours]

**Stereochemistry of polymers:** Geometric and optical isomerism in polymers. Structure, properties and preparation of stereoregular polymers.

Expressions for average molecular weights. Molecular weight distribution and Polydispersity.

**Determination of molecular weight:** Osmometry, viscometry, ultracentrifugation and GPC methods

**Thermal Characterization:** Glass Transition and melting-correlation with structure- Factors affecting  $T_g$  and  $T_m$ . Techniques of thermal characterization: DSC, DTA, DTG and TGA techniques.

### UNIT- III: [12 Hours]

**Structural features, properties and uses of commercial polymers:** polyethylene, polypropylene, polystyrene, PVC, polyesters, polyamides, polyurethanes and polycarbonates and regenerated cellulose.

**Properties and uses of Specialty polymers-** Composites, Conducting polymers and Biomedical polymers.

**Polymer degradation and stability-**thermal, oxidative, photo, chemical and radiation affected degradation. Plastic waste management-incineration, recycling and biodegradation.

**Polymer processing Techniques-**Compounding- role of additives. Casting, calendaring, moulding, foaming, reinforcing and spinning techniques.

### REFERENCES:-

1. Text book of Polymers- F.W. Billmeyer (Wiley)
2. Contemporary Polymer Chemistry-H.R. Allcock and F.W. Lampe (Prentice Hall).
3. Polymer Science and Technology-J.R. Frird (Prentice Hall).
4. Polymer Science: V.R. Gowariker, N.V. Viswanathan & T. Sreedhar
5. Principles of Polymer Science- P. Bahadur and N.V. Sastry (Narosa Publishers)

## CH S 556: NUCLEAR, RADIATION & PHOTOCHEMISTRY

### COURSE OUTCOME:

- The course content consists of two topics, radioactivity and various aspects of photochemical reactions.
- In the first part, the nuclear reactions, use of radioisotopes in analytical processes, design and functioning of nuclear reactors are taught along with the health and safety aspects of working with radiation.
- The second part deals with basic aspects of photochemical processes and their applications in synthesis, solar energy conversion,
- Understanding atmospheric reactions occurring in the presence of light.

### UNIT-I:

[12 Hours]

**Radioactivity and Nuclear Decay** –Nuclear stability-Liquid drop, shell and collective models Decay modes of natural and artificial nuclides- Determination of half life, growth kinetics. Conditions of equilibrium. Theories of  $\alpha$ ,  $\beta$  and  $\gamma$  emissions 4hrs

**Radiation Detection and Measurement:** Experimental techniques in the assay of radioactive isotopes. Radiation Detectors-ionisation chambers, proportional and Geiger-Muller, scintillation and semiconductor radiation detectors (NaI-Tl and Ge(Li), HPGGe solid state detectors). Liquid scintillators and multichannel analysers 4hrs

**Nuclear Reactions, Energy and Nuclear Power reactors** - Nuclear fission and fusion. Types of nuclear power reactors, basic features and components of a nuclear power reactor. An introduction to breeder reactors 4 hrs

### UNIT-II:

[12 Hours]

**Radioisotopes:-** Definition of curie and related calculations. Production of radioisotopes and labelled compounds by bombardment. Radiochemical separation techniques- carriers, solvent extraction and ion-exchange methods. Szilard-Chalmer process. Physico-chemical and analytical applications-isotope dilution method, activation analysis, radiometric titration and  $C^{14}$  dating. Medical, agricultural and industrial applications of isotopes. 5 hrs

**Radiation Chemistry:** Difference between radiation and photochemistry. Radiation sources, UNITS (LET, Rad, Roentgen and G-value), radiation dose and radiation chemical yield. Chemical Dosimetry-Fricke and ceric sulphate dosimeters. A brief introduction to radiolysis of gases, liquids and solids. Industrial applications of radiation chemistry (radiation synthesis, polymerization & food irradiation). 5hrs.

**Health and Safety Aspects:** Biological effects of radiation, Radiation protection, permissible exposure doses. Radioactive waste management. 2hrs

### UNIT-III:

[12 Hours]

#### Photochemistry

Introduction to photochemistry. Actinometry. Electronic energy states of atoms and molecules. - rules for transition between two energy states. Life time of excited electronic states. Franck-condon principle and its implications in predicting Absorption and Emission spectra. Absorption and emission spectra- effect of solute solvent interactions on electronic spectra-spectral shifts. Physicochemical properties of electronically excited molecules-excited state dipole moments, acidity constants. Photophysical pathways- Jablonski diagram.

Quenching-collisions in the gasphase, solution (Stern-Volmer equation) & by added substances 10hrs

A brief introduction to some current topics in photochemistry - Applications in synthesis, solar energy utilization and atmospheric photochemistry. 2hrs

#### REFERENCES:

1. Principles of Radiochemistry, Eds: Sood, Ramamoorthy & Reddy (IANCAS, BARC Mumbai)
2. Radiation Chemistry: An Overview, D.B. Naik and S. Dhanya (BARC, Mumbai)
3. Nuclear and Radiation Chemistry –Friedlander, Kennedy Macias & Miller (Wiley) 1981
4. Essentials of Nuclear Chemistry- H.J. Arnikaar (Wiley Eastern) 1987.
5. An Introduction to Radiation Chemistry, Spinks and Woods (Wiley, New York) 1990
6. Fundamentals of Photochemistry – Rohatgi and Mukherje (New Age Bangalore) 2000.



## CH P 557: INORGANIC CHEMISTRY PRACTICALS – IV

### COURSE OUTCOME:

- The students will have practical experience in determination of Na, K, Li and Ca by Flame photometry, Solvent extraction of Ni(II) and UO<sub>2</sub>(II),
- Preparation and analysis of complexes, Measurement of Magnetic susceptibility,
- Determination of composition of complexes by Job's method, Mole ratio method, Slope ratio method,
- Determination of stability constants by Turner Anderson method, Bejrrums method and Polarographic method.

1. Colorimetric determination of Ti(IV) and Zr(IV)
2. Simultaneous colorimetric determination of two metal ions – Mn and Cr.
3. Flame photometric determination of Na, K, Li and Ca individually and in mixtures.
4. Electrogravimetric determination of (a) Cu-Ni alloy and (b) Pb in Type Metal.
5. Solvent extraction of Ni(II) and UO<sub>2</sub>(II).
6. Preparation of any three of the following complexes, checking the purity of the prepared samples by chemicals analysis, structural study of the prepared complexes using conductance and magnetic susceptibility measurements, recording the electronic and infrared spectra:
  - i) Chloropentammincobalt(III) chloride, ii) Hexammincobalt(III)chloride.
  - iii) Potassium trisoxalatoferate(III) and iv) Potassium hexathiocyanatochromate(III)
  - v) K<sub>3</sub>Cr(OX)<sub>3</sub>.3H<sub>2</sub>O vi) Cu(tu)<sub>3</sub>Cl vii)Zn(tu)<sub>3</sub>OSO<sub>3</sub>
7. Determination of composition of complexes:
  - a) Job's method: Fe-phenanthroline complex
  - b) Mole ratio method: Zr-Alizarin red S complex,
  - c) Slope ratio method: Cu ethylenediamine complex,
  - d) Limiting logarithmic method: Uranyl-sulphosalicylic acid complex.
8. Determination of stability constants
  - a) Turner Anderson method: Fe-Tiron system,
  - b) Bejrrums's method: Cu – sulphosalicylic acid system,
  - c) Polarographic method: Cu-glycinate or Pb -oxalate system.

### REFERENCES:

1. J. Rose, Physicochemical Experiments
2. Vogel's Text Book of Quantitative Chemical Analysis (5<sup>th</sup> Ed), G.H. Jeffrey, J. Bassette, J. Mendham and R.C. Denny, Longman, 1999.

## CH P 558: PHYSICAL CHEMISTRY PRACTICALS-IV

### COURSE OUTCOME:

Includes large number of kinetic experiments from which students are made to choose five experiments which illustrate different principles of chemical kinetics. They are also expected to learn concepts of thermodynamics by carrying out 5 experiments from the respective section. The course also includes two experiments from polymer chemistry topics and two experiments from spectroscopy. In addition to the above knowledge, the students are trained to develop skill of using computers to draw chemical structures, to plot the data and to carry out calculations

### SPECIFIC COURSE OUTCOMES

- To Determine order of reaction order and activation parameters
- To study various types of reactions
- To determine the mechanism of reactions
- To study the catalytic constant, surface area of catalyst & temperature et.

#### A. Kinetics and Catalysis (Any Five Experiments are to be carried out)

Determination of reaction order and activation parameters, study of acidity/salt/solvent/catalytic effects on reaction rates of any FIVE of the reactions listed below.

1. Acid catalyzed hydrolysis of methyl acetate.
2. Saponification of ethyl acetate by conductivity method.
3. Decomposition of benzenediazonium chloride.
4. Reaction between potassium persulphate and potassium iodide (including the study of salt effect and catalysis by  $\text{Ag}^+$ ,  $\text{Fe}^{2+}$  and  $\text{Cu}^{2+}$  ions).
5. Decomposition of diacetone alcohol by NaOH & Hydrolysis of t-butylchloride.
6. (i) Reaction between iodine and acetone, and (ii) iodination of aniline.
7. Reaction between hydrogen peroxide and HI.
8. Decomposition of  $\text{H}_2\text{O}_2$  (including the study of catalytic effect).
9. Reaction between Chromic acid and oxalic acid.
10. Reduction of aqueous solution of ferric chloride by stannous chloride.
11. Determination of the mechanism of the oxidation of an organic compound from kinetic data.
12. Determination of catalytic constant of an acid.
13. Determination of effect of surface area of catalyst and temperature on the kinetics of Metal-acid reaction.
14. Determination of dissociation of trichloroacetic acid-Kinetic method.
15. Determination of equilibrium constant for homogeneous equilibria and determining the concentration of a given solution.
16. Determine the molecular formula of copper-ammonia complex by the partition coefficient method.
17. Alkaline hydrolysis of ethyl acetate volumetrically.
18. Effect of reaction surface area of catalyst and temperature, concentration on the kinetics of metal-acid

#### B. Polymer Chemistry (Any Two experiments are to be carried out)

1. Determination of molecular weight and size parameters of polymers by viscometry.
2. Determination of sequences in polyvinylalcohol by viscometry.
3. Determination of molecular weight of a polymer by turbidimetry.

4. Preparation of Polymethylmethacrylate by suspension polymerization / polystyrene by free radical polymerization / Nylon by interfacial polymerization / Polyacrylamide by solution polymerisation method / polyvinylalcohol from polyvinylacetate / Phenol formaldehyde/ urea formaldehyde resins / thin films of polymers.

### **C. Thermodynamics Experiments (Any Five experiments to be carried out)**

1. Determination of activities of an electrolyte and non-electrolyte by cryoscopy.
2. Determination of partial molar volumes of (a) Salts-water and (b) alcohol-water (methanol & ethanol) systems by density method.
3. Study of complex formation between mercury and potassium halides by cryoscopy.
4. Determination of specific heat of liquids and solutions by calorimetry.
5. Determination of stepwise neutralisation of acids.
6. Determination of heat of solution of  $\text{KNO}_3$  in water, integral heat of dilution of  $\text{H}_2\text{SO}_4$  and heat of ionization of acetic acid and ammonium hydroxide calorimetrically.
7. Cryoscopic and ebullioscopic analysis of the given mixture of urea and glucose.
8. Determination of vant Hoff's factor for benzoic and acetic acid mixtures in benzene.
9. Viscosity of sound in liquid-ultrasonic interferometry

### **D. Spectroscopic Experiments (Any Two experiments to be carried out)**

1. Kinetics of oxidation of alcohol by potassium dichromate – spectrophotometrically.
2. Simultaneous determination of Manganese and chromium in a solution of dichromate and Permanganate mixture.
3. Determination of pKa of an indicator..
4. Spectroscopic investigation of partition coefficient of iodine between  $\text{H}_2\text{O}$  and  $\text{CHCl}_3$ .
5. Study of the effect of ionic strength on the pH of the given acid with the help of indicators using buffer solution by colorimetric method.

**E. Computer related Practicals:** Solution of some selected chemical engineering problems to

develop skill for computer applications, programme writing and numerical analysis.

Use of commercial software packages such as Mathcad, Matlab, Aspan Plus, Design II, Use of Chem draw and Chem sketch for construction of molecules. Use of Window excel for drawing graphs estimation of slope intercept.



## CH P 559: PROJECT WORK AND DISSERTATION

### COURSE OUTCOME:

Enable the students:

- To design the project by collecting required background material by referring the literature
- To understand the functioning and safety features in the industry.
- To improve the experimental and soft skills.
- To learn various analytical and instrumental techniques and interpretation of analytical data.

