

# PONDICHERY UNIVERSITY

(A CENTRAL UNIVERSITY)



## **B.Sc. Chemistry**

(Choice Based Credit System)

Syllabus

2017-18 onwards

**Pondicherry University**  
**SCHEME FOR CHOICE BASED CREDIT SYSTEM**  
**B.Sc., Chemistry**  
**(With Effect from 2017-18 onwards)**

| COURSE   | SUBJECT CODE                                  | TITLE OF THE PAPER                                 | Credits           | Marks | Contact Hrs. / Week. | Lab Hrs. / Week |
|--|---|--|-------------------|-------|----------------------|-----------------|
| <b>SEMESTER-I</b>  |   |  | <b>18 Credits</b> |       |                      |                 |
| MIL – 1  | LBEN//LHIN/<br>LMAL/LSAN/<br>LTAM/LTEL<br>111 | Bengali/Hindi/Malayalam/<br>Sanskrit/Tamil/ Telugu | 03                | 100   | 03                   | -               |
| ENGLISH – 1  | ENGL 112                                      | ENGLISH – 1  | 03                | 100   | 03                   | -               |
| DSC – 1A   | UCHM 111                                      | General Chemistry – I                              | 04                | 100   | 04                   | -               |
| DSC – 2A   | UMAT 112                                      | Mathematics – I                                    | 04                | 100   | 04                   | -               |
|  | UZOO 112                                      | Zoology - I  | 03                | 75    | 03                   | -               |
| DSC – 3A   | UCHM 116                                      | General Chemistry Practical - I                    | 02                | 50    | -                    | 04              |
| DSC – 4A   | UZOO 116                                      | Zoology Lab - I                                    | 01                | 25    | -                    | 02              |
| AECC – 1   | PADM 111                                      | Public Administration                              | 02                | 50    | 02                   | -               |
| Note: Either UMAT 112 or UZOO 112 to be opted. UZOO 116 is only for UZOO 112 opted students. |   |  |                   |       |                      |                 |
| <b>SEMESTER-II</b>   |   |  | <b>18 Credits</b> |       |                      |                 |
| MIL – 2  | LBEN//LHIN/<br>LMAL/LSAN/<br>LTAM/LTEL<br>121 | Bengali/Hindi/Malayalam/<br>Sanskrit/Tamil/ Telugu | 03                | 100   | 03                   | -               |
| ENGLISH– 2   | ENGL 122                                      | ENGLISH – 2  | 03                | 100   | 03                   | -               |
| DSC – 1B   | UCHM 121                                      | General Chemistry-II                               | 04                | 100   | 04                   | -               |
| DSC – 2B   | UMAT 122                                      | Mathematics – II or                                | 04                | 100   | 04                   | -               |
|  | UZOO 122                                      | Zoology - II                                       | 03                | 75    | 03                   | -               |
| DSC – 3B   | UCHM 126                                      | General Chemistry Practical – II                   | 02                | 50    | -                    | 04              |
| DSC – 4B   | UZOO 126                                      | Zoology Lab - II                                   | 01                | 25    | -                    | 02              |
| AECC – 2   | ENVS 121                                      | Environmental Studies                              | 02                | 50    | 02                   | -               |
| Note: Either UMAT 122 or UZOO 122 to be opted. UZOO 126 is only for UZOO 122 opted students. |   |  |                   |       |                      |                 |
| <b>SEMESTER-III</b>  |   |  | <b>22 Credits</b> |       |                      |                 |
| MIL – 3  | LBEN//LHIN/<br>LMAL/LSAN/<br>LTAM/LTEL<br>231 | Bengali/Hindi/Malayalam/<br>Sanskrit/Tamil/ Telugu | 03                | 100   | 03                   | -               |
| ENGLISH – 3  | ENGL 232                                      | ENGLISH – III                                      | 03                | 100   | 03                   | -               |
| DSC – 1C   | UCHM 231                                      | Physical Chemistry - I                             | 04                | 100   | 03                   | -               |

|  |                                   |  |                   |     |    |    |
|--|-----------------------------------|--|-------------------|-----|----|----|
| DSC – 2C   | UCHM 232                          | Inorganic Chemistry - I                            | 04                | 100 | 03 | -  |
| DSC – 3C   | UPHY 233                          | Physics - I  | 03                | 75  | 03 | -  |
| DSC – 4C   | UCHM 236                          | Physical and Inorganic Chemistry - Practical       | 02                | 50  | -  | 04 |
| DSC – 5C   | UPHY 238                          | Physics Practical- I                               | 01                | 25  | -  | 02 |
| SEC – 1  | UCHM 234                          | IT Skills for Chemists                             | 02                | 50  | 01 | 02 |
| (Any One to be Selected)                         | UCHM 235                          | Basic Analytical Chemistry                         |                   |     |    |    |
|  | UCHM 237                          | Chemical Technology and Society                    |                   |     |    |    |
| <b>SEMESTER-IV</b>                               |                                   |  | <b>22 Credits</b> |     |    |    |
| MIL – 4  | LBEN/LHIN/LMAL/LSAN/LTAM/LTEL 241 | Bengali/Hindi/Malayalam/Sanskrit/Tamil/ Telugu     | 03                | 100 | 03 | -  |
| ENGLISH – 4                                      | ENGL 242                          | ENGLISH – IV                                       | 03                | 100 | 03 | -  |
| DSC – 1D   | UCHM 241                          | Physical Chemistry - II                            | 04                | 100 | 03 | -  |
| DSC – 2D   | UCHM 242                          | Organic Chemistry - I                              | 04                | 100 | 03 | -  |
| DSC – 3D   | UPHY 243                          | Physics - II                                       | 03                | 75  | 03 | -  |
| DSC – 4D   | UCHM 246                          | Physical and Organic Chemistry - Practical         | 02                | 50  | -  | 04 |
| DSC – 5D   | UPHY 248                          | Physics Practical- II                              | 01                | 25  | -  | 02 |
| SEC – 2  | UCHM 244                          | Analytical and Clinical Biochemistry               | 02                | 50  | 01 | 02 |
| (Any One to be Selected)                         | UCHM 245                          | Chemoinformatics                                   |                   |     |    |    |
|  | UCHM 247                          | Business Skills for Chemists                       |                   |     |    |    |
| <b>SEMESTER-V</b>                                |                                   |  | <b>20 Credits</b> |     |    |    |
| DSC – 1E   | UCHM 351                          | Inorganic Chemistry - II                           | 03                | 100 | 03 | -  |
| DSE – 1A<br>DSE – 2A<br>(Any Two to be Selected) | UCHM 352                          | Applications of Computers in Chemistry             | 04                | 75  | 04 | -  |
|  |                                   | Applications of Computers in Chemistry - Practical | 01                | 25  | -  | 02 |
|  | UCHM 353                          | Analytical Methods in Chemistry                    | 04                | 75  | 04 | -  |
|  |                                   | Analytical Methods in Chemistry: Practical         | 01                | 25  | -  | 02 |
|  | UCHM 354                          | Nano Chemistry                                     | 04                | 75  | 04 | -  |
|  |                                   | Nano Chemistry: Practical                          | 01                | 25  | -  | 02 |
|  | UCHM 355                          | Green Chemistry                                    | 04                | 75  | 04 | -  |

|  |          |   |                                 |     |    |                  |
|--|----------|---|---------------------------------|-----|----|------------------|
|  |          | Green Chemistry: Practical  | 01                              | 25  | -  | 02               |
|  | UCHM-356 | Organometallics, Bioinorganic Chemistry & Polynuclear hydrocarbons            | 04                              | 75  | 04 | -                |
|  |          | Organometallics, Bioinorganic Chemistry & Polynuclear hydrocarbons: Practical | 01                              | 25  | -  | 02               |
|  | UCHM-357 | Research Methodology  | 05                              | 100 | 05 | 02<br>(Tutorial) |
| DSC – 2E   | UCHM 350 | Inorganic Chemistry Practical - II  | 02                              | 50  | -  | 04               |
| GE – 1   | XXXX XXX | A course from other department  | 03                              | 100 | 03 | -                |
| SEC – 3<br>(Any One to be Selected)                        | UCHM 358 | Green Methods in Chemistry  | 02                              | 50  | 01 | 02               |
|  | UCHM 359 | Pharmaceutical Chemistry  |                                 |     |    |                  |
| <b>SEMESTER-VI</b>   |          |   | <b>20 Credits</b>               |     |    |                  |
| DSC – 1F   | UCHM 361 | Organic Chemistry - II  | 03                              | 100 | 03 | -                |
| DSE – 1B<br>DSE – 2B<br>(Any 2 DSE Courses to be selected) | UCHM 362 | Analytical Chemistry  | 04                              | 75  | 04 | 02               |
|  |          | Analytical Chemistry: Practical   | 01                              | 25  | -  | 02               |
|  | UCHM 363 | Polymer Chemistry   | 04                              | 75  | 04 | 02               |
|  |          | Polymer Chemistry: Practical  | 01                              | 25  | -  | 02               |
|  | UCHM 364 | Molecular Modelling & Drug Design   | 04                              | 75  | 04 | -                |
|  |          | Molecular Modelling & Drug Design:Practical                                   | 01                              | 25  | -  | 02               |
|  | UCHM 365 | Industrial Chemicals & Environment  | 04                              | 75  | 04 | -                |
|  |          | Industrial Chemicals & Environment: Practical                                 | 01                              | 25  | -  | 04               |
|  | UCHM 366 | Dissertation  | 05                              | 100 | -  | 10               |
|  | DSC – 2F | UCHM 360  | Organic Chemistry Practical -II | 02  | 50 | -                |
| GE – 2   | XXXX XXX | A course from other department  | 03                              | 100 | 03 | -                |
| SEC – 4<br>(Any One to be Selected)                        | UCHM 367 | Forensic Chemistry  | 02                              | 50  | 01 | 02               |
|  | UCHM 368 | Fuel Chemistry  |                                 |     |    |                  |

**Total Number of Credits: 120**

**Pondicherry University**  
**Syllabus for B. Sc., (Chemistry)**  
**Choice Based Credit System**

**I Year – Semester-I**

**DSC – IA: UCHM 111: GENERAL CHEMISTRY – I**

**Objective:**

**4-1-0-4**

- To Study Atomic Structure, Chemical Bonding and Molecular Structure
- To Study the Fundamentals of Organic Chemistry and Stereochemistry
- To Study the Gaseous state

**Unit – I: Atomic Structure**

Review of: Bohr's theory and its limitations, dual behaviour of matter and radiation, de Broglie's relation, Heisenberg Uncertainty principle. Hydrogen atom spectra. Need of a new approach to Atomic structure.

**Quantum mechanics:** Time independent Schrodinger equation and meaning of various terms in it. Significance of  $\psi$  and  $\psi^2$ , Schrödinger equation for hydrogen atom. Radial and angular parts of the hydronic wave functions (atomic orbitals) and their variations for 1s, 2s, 2p, 3s, 3p and 3d orbitals (Only graphical representation). Radial and angular nodes and their significance. Radial distribution functions and the concept of the most probable distance with special reference to 1s and 2s atomic orbitals. Significance of quantum numbers, orbital angular momentum quantum numbers  $m_l$  and  $m_s$ . Shapes of s, p and d atomic orbitals, nodal planes. Spin quantum number (s) and magnetic spin quantum number ( $m_s$ ).

**(12 Lectures)**

**Unit II: Chemical Bonding and Molecular Structure**

**Ionic Bonding:** General characteristics of ionic bonding. Energy considerations in ionic bonding, Lattice energy and solvation energy and their importance in the context of stability and solubility of ionic compounds. Statement of Born-Landé equation for calculation of lattice energy, Born-Haber cycle and its applications, polarizing power and polarizability. Fajan's rules, ionic character in covalent compounds, bond moment, dipole moment and percentage ionic character.

Covalent bonding: VB Approach: Shapes of some inorganic molecules and ions on the basis of VSEPR and hybridization with the following examples –  $\text{BeCl}_2$ ,  $\text{BF}_3$ ,  $\text{NH}_3$ ,  $\text{SF}_4$ ,  $\text{PCl}_5$ ,  $\text{SF}_6$ .

Concept of resonance and resonating structures in various inorganic compounds. MO Approach: Rules for the LCAO method, bonding and anti-bonding MOs and their characteristics for s-s, s-p and p-p combinations of atomic orbitals, MO treatment of homonuclear diatomic molecules of  $\text{O}_2$  and  $\text{N}_2$  and heteronuclear diatomic molecules such as CO, NO and  $\text{NO}^+$ . Comparison of VB and MO approaches.

**(12 Lectures)**

### Unit III: Fundamentals of Organic Chemistry

Physical Effects, Electronic Displacements: Inductive Effect, Electromeric Effect, Resonance and Hyperconjugation. Cleavage of Bonds: Homolysis and Heterolysis.

Structure, shape and reactivity of organic molecules: Nucleophiles and electrophiles. Reactive Intermediates: Carbocations, Carbanions and free radicals.

Strength of organic acids and bases: Comparative study with emphasis on factors affecting pK values. Aromaticity: Benzenoids and Hückel's rule.

Introduction to types of organic reactions: Addition, Elimination and Substitution reactions.

(12 Lectures)

### Unit IV: Stereochemistry

Conformations with respect to ethane, butane and cyclohexane. Interconversion of Wedge Formula, Newmann, Sawhorse and Fischer representations. Concept of chirality (up to two carbon atoms). Configuration: Geometrical and Optical isomerism; Enantiomerism, Diastereomerism and Meso compounds). Threo and erythro; D and L; cis - trans nomenclature; CIP Rules: R/ S (for upto 2 chiral carbon atoms) and E / Z Nomenclature (for upto two C=C systems).

(12 Lectures)

### Unit V: Gaseous State:

**Kinetic molecular model of a gas:** Postulates and derivation of the kinetic gas equation - collision frequency - collision diameter - mean free path and viscosity of gases, including their temperature and pressure dependence, relation between mean free path and coefficient of viscosity, calculation of  $\sigma$  from  $\eta$ ; variation of viscosity with temperature and pressure. Maxwell distribution and its use in evaluating molecular velocities (average, root mean square and most probable) and average kinetic energy, law of equipartition of energy, degree of freedom and molecular basis of heat capacities.

**Behaviour of real gases:** Deviations from ideal gas behaviour, compressibility factor, Z and its variation with pressure and temperature for different gases. Causes of deviation from ideal behaviour. van der Waals equation of state, its derivation and application in explaining real gas behaviour, calculation of Boyle temperature. Isotherms of real gases and their comparison with van der Waals isotherms, continuity of states, critical state, relation between critical constants and van der Waals constants, law of corresponding states.

(12 Lectures)

### Reference Books:

- Lee, J.D. Concise Inorganic Chemistry ELBS, 1991.
- Cotton, F.A., Wilkinson, G. & Gaus, P.L. Basic Inorganic Chemistry, 3<sup>rd</sup> Ed., Wiley.
- Douglas, B.E., McDaniel, D.H. & Alexander, J.J. Concepts and Models in Inorganic Chemistry, John Wiley & Sons.

- Huheey, J.E., Keiter, E.A., Keiter, R.L. & Medhi, O.K. Inorganic Chemistry: Principles of Structure and Reactivity, Pearson Education India, 2006.
- Graham Solomon, T.W., Fryhle, C.B. & Snyder, S.A. Organic Chemistry, John Wiley & Sons (2014).
- McMurry, J.E. Fundamentals of Organic Chemistry, 7<sup>th</sup> Ed. Cengage Learning India Edition, 2013.
- Sykes, P. A Guidebook to Mechanism in Organic Chemistry, Orient Longman, New Delhi (1988).
- Eliel, E.L. Stereochemistry of Carbon Compounds, Tata McGraw Hill education, 2000.
- Finar, I.L. Organic Chemistry (Vol. I & II), E.L.B.S.
- Morrison, R.T. & Boyd, R.N. Organic Chemistry, Pearson, 2010.
- Bahl, A. & Bahl, B.S. Advanced Organic Chemistry, S. Chand, 2010.
- Puri B.R., Sharma L.R. and Kalia K.C. Principles of Inorganic Chemistry, Milestone.
- Arun Bahl, Bahl, B.S. and Tuli G.D. *Essentials of Physical Chemistry*, S. Chand & Co, 2012.
- Peter Atkins and Julio de Paula, *Atkin's Physical Chemistry* 9<sup>th</sup> Ed., Oxford University Press.
- Puri B.R., Sharma L.R. and Pathania M.S. *Principles of Physical Chemistry*, Vishal Publishing Co., 2008.

## DSC-3A: UCHM 116: GENERAL CHEMISTRY PRACTICAL – I

(60 Lectures)

0-1-4-2

### Volumetric Analysis & Chromatography

1. Preparation of standard solutions of different Molarities and Normalities.
2. Estimation of sodium carbonate and sodium hydrogen carbonate present in a mixture.
3. Estimation of oxalic acid by preparing standard FAS and titrating it with  $\text{KMnO}_4$ .
4. Estimation of  $\text{Fe}^{2+}$  by preparing standard FAS and using  $\text{KMnO}_4$  link solution.
5. Estimation of water of crystallization in Mohr's salt by titrating with  $\text{KMnO}_4$ .
6. Estimation of Fe (II) ions by titrating it with  $\text{K}_2\text{Cr}_2\text{O}_7$  using internal indicator.
7. Estimation of  $\text{K}_2\text{Cr}_2\text{O}_7$  iodometrically by preparing standard  $\text{K}_2\text{Cr}_2\text{O}_7$  and link  $\text{Na}_2\text{S}_2\text{O}_3$ .
8. Estimation of Cu (II) ions iodometrically by preparing standard  $\text{CuSO}_4$  and link  $\text{Na}_2\text{S}_2\text{O}_3$ .
9. Separation of mixtures by Chromatography: Measure the  $R_f$  value in each case (combination of two compounds to be given)
10. Identify and separate the components of a given mixture of two amino acids (glycine, aspartic acid, glutamic acid, tyrosine or any other amino acid) by paper chromatography
11. Identify and separate the sugars present in the given mixture by paper chromatography.

### Reference Books:

- Svehla, G. Vogel's Qualitative Inorganic Analysis, Pearson Education, 2012.
- Mendham, J. Vogel's Quantitative Chemical Analysis, Pearson, 2009.
- Vogel, A.I., Tatchell, A.R., Furnis, B.S., Hannaford, A.J. & Smith, P.W.G.,  
Textbook of Practical Organic Chemistry, Prentice-Hall, 5<sup>th</sup> edition, 1996.
- Mann, F.G. & Saunders, B.C. Practical Organic Chemistry Orient-Longman, 1960.

### Scheme of Valuation: (Max marks: 50)

|   |       |                      |
|---|-------|----------------------|
| 1. Internal Marks                         | ----- | 10 marks             |
| 2. Writing Principle and brief procedure  | ----- | 5 marks              |
| 3. Record                                 | ----- | 5 marks              |
| 4. Viva-voce                              | ----- | 5 marks              |
| 5. Experiment (based on error %)          | ----- | 25 marks (see below) |
| Up to 2% error                            | ----- | 25 marks             |
| 2% to 3%                                  | ----- | 20 marks             |
| 3% to 4%                                  | ----- | 15 marks             |
| 4% to 5%                                  | ----- | 10 marks             |
| More than 5% error or expt. is incomplete | ----- | 5 marks              |

For calculation mistake: 2 marks to be deducted; for no calculation: 5 marks to be deducted.



## I Year - Semester - II

### DSC- 1B: UCHM 121: GENERAL CHEMISTRY-II

(60 Lectures)

4-1-0-4

#### Objective:

- To Study Chemical Energetics
- To Study the Chemical Equilibrium, Ionic Equilibria
- To Study the Hydrogen, Hydrides, and S-block elements
- To Study the Aliphatic Hydrocarbons, Aromatic Hydrocarbons

#### Unit I: Chemical Energetics

Review of thermodynamics and the Laws of Thermodynamics.

Important principles and definitions of thermochemistry. Concept of standard state and standard enthalpies of formations, integral and differential enthalpies of solution and dilution. Calculation of bond energy, bond dissociation energy and resonance energy from thermochemical data. Variation of enthalpy of a reaction with temperature – Kirchhoff's equation.

#### Third law of thermodynamics:

Statement of third law; concept of residual entropy; Nernst heat theorem; Evaluation of absolute entropy from heat capacity data.

(12 Lectures)

#### Unit II: Chemical Equilibrium & Ionic Equilibria:

Free energy change in a chemical reaction. Thermodynamic derivation of the law of chemical equilibrium. Distinction between  $\Delta G$  and  $\Delta G^\circ$ , Le Chatelier's principle. Relationships between  $K_p$ ,  $K_c$  and  $K_x$  for reactions involving ideal gases.

Strong, moderate and weak electrolytes, degree of ionization, factors affecting degree of ionization, ionization constant and ionic product of water. Ionization of weak acids and bases, pH scale, common ion effect. Salt hydrolysis-calculation of hydrolysis constant, degree of hydrolysis and pH for different salts. Buffer solutions. Solubility and solubility product of sparingly soluble salts – applications of solubility product principle.

(12 Lectures)

#### Unit III: Hydrogen, Hydrides, and S-block elements

Hydrogen-Isotopes, ortho- and para-hydrogens. Hydrides: ionic, covalent, metallic and interstitial hydrides, Hydrogen bonding.

Alkali metals: Introduction, halides, oxides and hydroxides, salts of oxo-acids, aqueous solution chemistry, complexes and organometallic compounds.

Alkaline Earth metals: Introduction, halides, oxides and hydroxides, salts of oxo-acids, aqueous solution chemistry, complexes and organometallic compounds.

(12 Lectures)

#### Unit IV: Aliphatic Hydrocarbons

**Alkanes:** Preparation – Catalytic hydrogenation, Wurtz reaction, Kolbe's synthesis, from Grignard reagent. **Reactions:** Free radical Substitution: Halogenation.

**Cycloalkanes:** Preparation by Dieckman condensation & Baeyer's strain theory. Conformational analysis of mono- and di-substituted cyclohexanes.

**Alkenes:** Preparation – Elimination reactions: Dehydration of alkenes and dehydrohalogenation of alkyl halides (Saytzeff's rule); *cis*-alkenes (Partial catalytic hydrogenation) and *trans*-alkenes (Birch reduction). **Reactions:** *cis*-addition (alkaline  $\text{KMnO}_4$ ) and *trans*-addition (bromine), addition of HX (Markownikoff's and anti-Markownikoff's addition), hydration, ozonolysis, oxymecuration-demercuration, hydroboration-oxidation.

**Alkynes:** Preparation of acetylene from  $\text{CaC}_2$  and conversion into higher alkynes by dehalogenation of tetra halides and dehydrohalogenation of vicinal-dihalides.

**Reactions:** Formation of metal acetylides, addition of bromine and alkaline  $\text{KMnO}_4$ , ozonolysis and oxidation with hot alkaline  $\text{KMnO}_4$ .

(12 Lectures)

#### Unit V: Aromatic Hydrocarbons

Preparation (Case benzene): from phenol, by decarboxylation, from acetylene, from benzene sulphonic acid.

Reactions: (Case benzene): Electrophilic substitution: nitration, halogenation and sulphonation. Friedel-Craft's reaction (alkylation and acylation) (up to 4 carbons on benzene). Side chain oxidation of alkyl benzenes (up to 4 carbons on benzene).

Activating and deactivating substituents. Orientation and ortho-para ratio. Addition reactions of benzene - Birch reduction.

(12 Lectures)

#### Reference Books:

- Huheey, J.E., Keiter, E.A., Keiter, R. L., Medhi, O.K. Inorganic Chemistry, Principles of Structure and Reactivity, Pearson Education 2006.
- Lee, J.D. Concise Inorganic Chemistry, John Wiley & Sons.
- Graham Solomon, T.W., Fryhle, C.B. & Snyder, S.A. Organic Chemistry, John Wiley & Sons (2014).
- McMurry, J.E. Fundamentals of Organic Chemistry, 7th Ed. Cengage Learning India Edition, 2013.
- Arun Bahl and Bahl, B.S. Advanced Organic Chemistry, S. Chand & Co. Ltd., 2012.
- Arun Bahl, Bahl, B.S. and Tuli G.D. Essentials of Physical Chemistry, S. Chand & Co, 2012.
- Peter Atkins and Julio de Paula, Atkin's Physical Chemistry 9th Ed., Oxford University Press.
- Puri B.R., Sharma L.R. and Pathania M.S. Principles of Physical Chemistry, Vishal Publishing Co., 2008.
- Hari Jeevan Arnikar, Essentials of Nuclear Chemistry, Revised 4th Ed., New Age International Publishing, 1995.

## DSC - 3B: UCHM 126: GENERAL CHEMISTRY PRACTICAL – II

(60 Lectures)

0-1-4-2

### Physical Chemistry Experiments

1. Determination of heat capacity of calorimeter for different volumes.
2. Determination of enthalpy of neutralization of hydrochloric acid with sodium hydroxide.
3. Determination of enthalpy of ionization of acetic acid.
4. Determination of integral enthalpy of solution of salts ( $\text{KNO}_3$ ,  $\text{NH}_4\text{Cl}$ ).
5. Determination of enthalpy of hydration of copper sulphate.
6. Study of the solubility of benzoic acid in water and determination of  $\Delta H$ .
7. Determination of molecular mass by Rast's macro method.
8. Determination of transition temperature of the given substance by thermometric method ( $\text{Na}_2\text{S}_2\text{O}_3 \cdot 5\text{H}_2\text{O}$ ;  $\text{SrCl}_2 \cdot 6\text{H}_2\text{O}$ ;  $\text{CH}_3\text{COONa} \cdot 3\text{H}_2\text{O}$ ;  $\text{MnCl}_2 \cdot 4\text{H}_2\text{O}$ )
9. Distribution coefficient of iodine between water and carbon tetrachloride.
10. Construction of the phase diagram of a binary system (simple eutectic) using cooling curves.
11. Determination of the critical solution temperature (CST) and composition of the phenol water system.
12. Effect of added electrolytes on the miscibility temperature of phenol-water system.

### Reference Books:

1. Svehla, G. Vogel's Qualitative Inorganic Analysis, Pearson Education, 2012.
2. Mendham, J. Vogel's Quantitative Chemical Analysis, Pearson, 2009.
3. Vogel, A.I., Tatchell, A.R., Furnis, B.S., Hannaford, A.J. & Smith, P.W.G., Textbook of Practical Organic Chemistry, Prentice-Hall, 5<sup>th</sup> edition, 1996.
4. Mann, F.G. & Saunders, B.C. Practical Organic Chemistry. Pearson Education (2009).
5. Khosla, B. D.; Garg, V. C. & Gulati, A. Senior Practical Physical Chemistry, R. Chand & Co., New Delhi (2011).

### Scheme of Valuation: (Max marks: 50)

- |   |                            |
|---|----------------------------|
| 1. Internal Marks   | ----- 10 marks             |
| 2. Writing principle, formula/graph, etc.                     | ----- 5 marks              |
| 3. Record   | ----- 5 marks              |
| 4. Viva-voce  | ----- 5 marks              |
| 5. Experiment (based on error % with theoretical value) ----- | 25 marks (see below)       |
| Up to 2% error  | ----- 25 marks             |
| 2% to 3%  | ----- 20 marks             |
| 3% to 4%  | ----- 15 marks             |
| 4% to 5%  | ----- 10 marks             |
| More than 5% error or expt. is incomplete                     | ----- 5 marks (grace mark) |
- For calculation mistake: 2 marks to be deduced; For no calculation: 5 marks to be deduced.

## II Year – Semester - III

### DSC-IC: UCHM 231: PHYSICAL CHEMISTRY – I

3-1-0-3

#### Objective:

- To Study the Solid State and X-ray diffraction studies.
- To Study the Chemical Kinetics
- To Study the Catalysis, Adsorption and Photochemistry.
- To Study the Dilute Solutions and Colligative Properties.
- To Study the Phase Equilibrium.

#### UNIT – I SOLID STATE (12 Hours)

- (a) Definition of Space lattice , Unit cell , Laws of crystallography –
- (i) Law of constancy of interfacial angles
  - (ii) Law of rationality of indices
  - (iii) Law of symmetry, symmetry elements in crystals
- (b) X-ray diffraction by crystals -- Derivation of Bragg's equation. Determination of structures of NaCl, CsCl, KCl, (Laue's method and powder method).

#### UNIT-II CHEMICAL KINETICS (12 Hours)

Rate and specific reaction rate; Factors influencing the rate of reaction-concentration, temperature, pressure, catalyst, solvent and light; Order and Molecularity of reactions; Derivation of rate constants-zero, first and second order (with equal and unequal concentrations) reactions; Half-life period; Pseudo order reactions; Determination of order of reactions-differential method, method of integration and method of half-life period.

Effect of temperature on reaction rate; Arrhenius equation; Activation energy and its significance; Theory of reactions-Collision theory and Transition state theory.

#### UNIT-III CATALYSIS, ADSORPTION AND PHOTOCHEMISTRY (12 Hours)

##### (a) CATALYSIS

Catalyst and catalysis: Homogeneous and heterogeneous catalysis with examples; Acid-base catalysis with examples; Enzyme catalysis-general characteristics; Auto catalysis; Derivation of Michaelis-Menten constant. Theories of catalysis-intermediate compound formation theory and adsorption theory.

### **(b) ADSORPTION**

Adsorption-physisorption and chemisorptions; Factors influencing adsorption; Adsorption Isotherms-Freundlich, Langmuir and BET theories. Application of adsorptions.

### **(c) PHOTOCHEMISTRY**

Difference between thermal and photochemical reactions; Laws of photochemistry-Grothus-Drapper and Stark-Einstein laws; Jablonski diagram; qualitative description of fluorescence and phosphorescence; Non-radiative processes –internal conversion and inter system crossing; Quantum yield.

## **UNIT-IV DILUTE SOLUTIONS AND COLLIGATIVE PROPERTIES (12 Hours)**

Method of expressing concentrations of solutions; dilute solutions; colligative properties; Raoult's law; relative lowering of vapour pressure; Molecular weight determination; Law of osmotic pressure; determination molecular weight by osmotic pressure; elevation of boiling point and depression of freezing point; thermodynamic derivation of the relation between molecular weight and elevation of boiling point and the relation between molecular weight and depression of freezing point.

## **UNIT-V PHASE EQUILIBRIUM (12 Hours)**

Definition of Phase, Component and Degrees of Freedom; Derivation of Gibb's phase rule; Phase equilibria of one component systems –  $H_2O$ ,  $CO_2$  and sulphur systems; Two component systems – Solid-Liquid equilibria- simple eutectic Bi-Cd and Pb-Ag systems; desilverisation of lead; Solid solutions-compound formation with congruent melting point (Mg-Zn) and incongruent melting point ( $NaCl-H_2O$  and  $CuSO_4-H_2O$ ) systems.

Liquid-liquid mixtures-ideal liquid mixtures; Raoult's and Hendry's law; non-ideal solutions; partially miscible liquids-phenol-water; trimethylamine-water and nicotin-water systems. Lower and upper consolute temperature. Effect of impurity on consolute temperature.

Azeotropes- $HCl-H_2O$  and ethanol-water systems.

Nernst distribution law-thermodynamic derivations and applications.

### **Text Books**

1. S.H. Maron and J.B. Lando, *Fundamentals of Physical Chemistry*, Macmillan limited, New York, 1966.
2. B.R. Puri, L.R. Sharma and M.S. Pathania, *Principles of Physical Chemistry*, 46th Edition, Vishal Publishing Company, New Delhi, 2013.
3. Gurdeep Raj, *Advanced Physical Chemistry*, 35<sup>th</sup> Edition, Goel Publishing House, Meerut, 2009.
4. P.W. Atkins, *Physical Chemistry*, 7th edition, Oxford university press, 2001.
5. S.K. Dogra and S. Dogra, *Physical Chemistry Through Problems*, New age international, 4th edition 1996.

### **Reference Books**

1. Gilbert. W. Castellan, *Physical Chemistry*, Narosa publishing house, third edition 1985.
2. Irving M. Klotz and Robert M. Rosenberg, *Chemical Thermodynamics*, John Wiley and sons, Inc. 1994.
3. J. Rajaram and J.C. Kuriacose, *Thermodynamics*, Shoban Lal Nagin Chand and CO. 1986.
4. K. L. Kapoor, *A Textbook of Physical chemistry*, (volume-2 and 3) Macmillan, India Ltd, 1994.
5. K. Laidler, *Chemical Kinetics*, 3rd Edition, Pearson Education, New Delhi, 2004.
6. K.K. Sharma and L.K. Sharma, *A Textbook of Physical Chemistry*, 5th Edition, Vikas Publishing House, New Delhi, 2012.
7. K.L. Kapoor, *Physical Chemistry Vol. 3&5*, Macmillan Publishers, Noida, 2004.
8. G.K. Vemula Palli, *Physical Chemistry*, Prentice Hall of India, New Delhi, 1997.

## II Year – Semester - III

### DSC-2C: UCHM 232: INORGANIC CHEMISTRY-I

3-1-0-3

#### Objective:

- To Study Nuclear Chemistry
- To Study the Principles of Qualitative Inorganic Analysis
- To Study the Theories of Acids, Bases & Non-aqueous solvents
- To Study the P-Block Elements

#### UNIT – I: NUCLEAR CHEMISTRY

(12 Hrs)

Nuclear forces- atomic mass unit- packing fraction – mass defect and binding energy of the nucleus. Stability of nuclei. Nuclear models- the liquid drop model. Nuclear reactions- nuclear fission- fission of uranium- nuclear reactors- types- importance of thorium in India's nuclear energy production. Nuclear fusion. Radio activity- natural radio activity- rate of radio activity disintegration – half life period- transmutation of elements- group displacement law- radio active decay series. Isotopes-separation of isotopes - applications of isotopes in analytical chemistry, medicine, and in reaction mechanism. Carbon dating. Neutron activation analysis. (12 Hrs)

#### UNIT-II: PRINCIPLES OF QUALITATIVE INORGANIC ANALYSIS (12 Hrs)

(a) Principles of solubility – solubility product – factors affecting solubility – temperature, solvent, common ion effect, effect of complex formation – Separation of metal ions based on solubility differences – sulphide separations. Applications of solubility product principle in qualitative and quantitative analysis. Standard semi micro procedure of identifying common anions and cations in a mixture containing two salts. Spot tests for common cations. Interfering radicals – reason for their interference and method of their removal.

(b) Techniques of separation and purification of mixtures -gravity and suction filtration – centrifugation- drying techniques-melting point and boiling point determinations.

#### UNIT-III: ACIDS, BASES & NON-AQUEOUS SOLVENTS (12 Hrs)

(a) Acids and Bases-Bronsted acids and bases: Lewis acids and bases: definitions, strengths, representative Lewis acids, heterogeneous acid-base reactions.

Hard & soft acids & bases (HSAB) : Classification, Pearson's HSAB concept, acid basestrength & hardness and softness.

(b) Physical properties of a solvent, Types of solvents and their general characteristics. Reactions in non-aqueous solvents with reference to liquid  $\text{NH}_3$  and liquid  $\text{SO}_2$ , THF and Dioxan.

#### **UNIT-IV: P-BLOCK ELEMENTS –I (Boron, Carbon and Nitrogen group) (12 Hrs)**

(a) General characteristics of Boron group elements - Diagonal relationship between B and Si. Hydrides of Boron – preparation, properties and structure of Diborane. Boron Nitride, Borazine, Sodium Borohydride and Lithium Aluminium hydride, Boric acid

(b) General characteristics of carbon group elements – Allotropy of carbon, structure of Diamond and Graphite, catenation, fullerenes. Fluorochlorocarbons, silicates and carbides.

c) General characteristics of Nitrogen group elements. Allotropy of phosphorus, oxides ( $\text{N}_2\text{O}$ ,  $\text{NO}_2$ ,  $\text{N}_2\text{O}_3$ ,  $\text{N}_2\text{O}_5$ ,  $\text{P}_2\text{O}_3$ ,  $\text{P}_2\text{O}_5$ ) and Acids of Nitrogen ( $\text{HNO}_2$ ,  $\text{HNO}_3$ ) & Phosphorus ( $\text{H}_3\text{PO}_3$ ,  $\text{H}_3\text{PO}_4$ ,  $\text{H}_4\text{P}_2\text{O}_7$ ). Preparation and Structure and uses of Hydrazine, Hydrazoic acid and Hydroxylamine.

#### **UNIT-IV: P-BLOCK ELEMENTS –II ( Oxygen, Halogens and noble gases group)**

**(12 Hrs)**

(a) General characteristics of Oxygen group. Allotropy of sulphur - oxides, halides, oxyhalides of sulphur. Oxyacids ( $\text{H}_2\text{SO}_4$ ,  $\text{H}_2\text{SO}_3$ ,  $\text{H}_2\text{S}_2\text{O}_7$ ) of sulphur. Persulphuric acids, Dithionic and Thiosulphuric acid (structure, preparation and properties).

(b) General characteristics of halogen group elements, Oxides and oxoacids of halogens, Relative strength of oxo acids of the halogens, inter halogen compounds, Pseudo halogens, Electro positive character of iodine.

c) Chemistry of noble gases:- Position in the periodic table. Occurrence- isolation and separation of noble gases from atmosphere. Physical properties of noble gases, fluorides- oxyfluorides and oxides of xenon (preparation, properties and structure). Applications of noble gases.

#### **Reference Books:**

1. Cotton, F.A., Wilkinson, G. & Gaus, P.L. Basic Inorganic Chemistry, 3<sup>rd</sup> Ed., Wiley.
2. Douglas, B.E., McDaniel, D.H. & Alexander, J.J. Concepts and Models in Inorganic Chemistry, John Wiley & Sons.
3. Puri B.R., Sharma L.R. and Kalia K.C. Principles of Inorganic Chemistry, Milestone



4. Huheey, J.E., Keiter, E.A., Keiter, R. L., Medhi, O.K. Inorganic Chemistry, Principles of Structure and Reactivity, Pearson Education 2006.
5. Lee, J.D. Concise Inorganic Chemistry, John Wiley & Sons.
6. HariJeevanArnikar, Essentials of Nuclear Chemistry, Revised 4th Ed., New Age International Publishing, 1995.
7. Rodgers, G.E. Inorganic & Solid State Chemistry, Cengage Learning India Ltd., 2008. Miessler, G. L. & Donald, A. Tarr. Inorganic Chemistry 4<sup>th</sup> Ed., Pearson, 2010.
8. Atkin, P. Shriver & Atkins' Inorganic Chemistry 5<sup>th</sup> Ed. Oxford University Press (2010).

## DSC-4C: UCHM 236: PHYSICAL AND INORGANIC CHEMISTRY PRACTICAL

(60 Lectures)

0-1-4-2

### A. Physical Chemistry

Surface tension and Viscosity measurements (use of organic solvents excluded).

1. Determination of the surface tension of the given liquid or dilute solution using a stalagmometer.
2. Determination of the viscosity of the given liquid or dilute solution using an Ostwald's viscometer.
3. Determination of m.pt of the given compound using water bath (m.pt.< 100° C)

### B. Inorganic Chemistry

Systematic semi-micro qualitative analysis of mixtures - not more than four ionic species (two anions and two cations, excluding insoluble salts) out of which one anion being an interfering radical:

**Cations:** Lead, antimony, arsenic, tin, bismuth, cadmium, copper, aluminium, chromium, iron, manganese, zinc, nickel, cobalt, calcium, strontium, barium, magnesium, potassium and ammonium.

**Anions:** Carbonate, sulphide, chloride, bromide, iodide, sulphate, nitrate, phosphate, borate, oxalate, acetate and fluoride.

(using H<sub>2</sub>S or other methods. Spot tests should be carried out wherever feasible).

**(Combination of mixtures forming insoluble salts should be avoided)**

### Reference Books:

Svehla, G. Vogel's Qualitative Inorganic Analysis, Pearson Education, 2012.

J. Mendham, R.C. Denney, J. D. Barnes, M.J.K. Thomas, Vogel's Quantitative Chemical Analysis, Pearson, 2009.

Khosla, B. D.; Garg, V. C. & Gulati, A. Senior Practical Physical Chemistry, R. Chand & Co.: New Delhi (2011)

### Scheme of Valuation: (Max marks: 50)

- |  |       |          |
|--|-------|----------|
| 1. Internal Marks                        | ----- | 10 marks |
| 2. Record (containing both A & B)        | ----- | 10 marks |
| 3. Any one Physical Chemistry Experiment | ----- | 5 marks  |
| 4. Inorganic Qualitative Analysis        | ----- | 25 marks |

## II – Year – Semester - III

### SEC-1: UCHM234: IT SKILLS FOR CHEMISTS

(30 Lectures)

1-1-0-2

#### Objectives:

- To introduce the basics of computers.
- To learn C language and its applications in solving problems in Chemistry.

#### Unit-I

**Introduction:** Basic computer organization, processor and memory – main memory, secondary storage devices and storage hierarchy. Software – relationship between hardware and software – types of software. Planning the computer program – algorithm and flowcharts. Basics of operating systems.

#### Unit-II

**Computer languages** – machine language, assembly language, assembler, compiler, interpreter and programming languages - C language – introduction, C compiler, operating systems and preprocessor directives - variables, constants, operators, input and output functions.

#### Unit-III

**Control structures** – conditional, looping, goto, break, switch and continue statements, functions, arrays and pointers.

#### Unit-IV

**Applications in Chemistry-I** – calculation of the radius of the first Bohr orbit for an electron, calculation of half-life time for an integral order reaction, calculation of molarity, molality and normality of a solution, calculation of pressure of ideal or Vanderwaal's gas, Calculation of electronegativity of an element using Pauling's relation.

#### Unit-V

**Applications in Chemistry-II** - Calculation of empirical formulae of hydro carbon, calculation of reduced mass of a few diatomic molecules, determination of the wave numbers of spectral lines of hydrogen atom, calculation of work of expansion in adiabatic process, calculation of pH, solubility product and bond energy using Born - Lande equation, calculation of standard deviation and correlation coefficient.

## **PRACTICALS (FOR INTERNAL ASSESSMENT ONLY):**

Learning activities and evaluation of skills in using the following:

- Computer software and data logging equipment in chemistry.
- Portable ICT devices for modelling and simulation
- Worksheet, spreadsheet, database templates and graph drawing software
- Web-based resources: for interacting with appropriate teaching and learning chemistry
- Learning chemistry materials on CD-ROMs, websites and interactive multi-media display boards

**Students will perform four to five experiments based on topics that are covered in the Units IV and V.**

## **SCHEME OF EXAMINATION:**

|                               |       |  |
|-------------------------------|-------|--|
| External Theory Examination   | ----- | <b>40 marks</b> (to be conducted by University with time duration of 2 Hrs.)   |
| Internal Practical Assessment | ----- | <b>10 marks</b> (to be provided by the teacher as CIA, based on the performance of students in acquiring the skills) |

## **Reference Books:**

1. K.V. Raman, Computers in Chemistry, 8<sup>th</sup> Edition, Tata McGraw Hill, 2005.
2. Venugopal and Prasad, Programming with C, 11<sup>th</sup> Edition, 1971.
3. Balaguruswamy, Programming in C, 2<sup>nd</sup> Edition, 1989.

## II – Year – Semester - III

### SEC-1: UCHM235: BASIC ANALYTICAL CHEMISTRY

(30 Lectures)

1-1-0-2

#### UNIT-I

(10 Hrs)

##### **(A) Laboratory Glassware:**

- Types, maintenance and cleaning.
- Calibration of burette, pipette and standard flask; practice of inter-calibration.
- Laboratory first aids.

##### **(B) Stoichiometry and concentration systems:**

Stoichiometry – Mole and equivalent concepts – Stoichiometric calculations - concentration systems – Molarity – Normality – p-functions – percent concentration – ppm and ppb - calculations involving various types of concentration systems.

#### UNIT-II

(10 Hrs)

##### **Principles of Titrimetric (Volumetric) Analysis:**

- Definition of the terms primary standard and secondary standard solutions — Equivalence point and end point of titrations, — Types of titrations — Calculations involving volumetric titrations.
- Acid - Base Titrations : Derivation of titration curves for strong acid Vs strong base and weak acid Vs strong base titrations — Theory of acid-base indicators.
- Redox Titrations : Nernst equation — Theory of redox indicators — Types of redox indicators.
- Complex Formation Titrations: Chelating agents – EDTA- Theory of metallochromic indicators – Titrations involving EDTA – Types of EDTA titrations.
- Precipitation Titrations: Argentometric titrations – indicators for titrations involving silver nitrate.

#### UNIT-III

(10 Hrs)

##### **Statistical Evaluation of Analytical Data :**

Mean, median and mode – Accuracy and precision – ways of expressing accuracy and precision and their calculation – Errors – types – determinate, indeterminate and gross errors – minimization of errors – methods of reporting data – significant figures and problems involving significant figures – Statistical treatment of indeterminate errors – confidence limits – criteria for rejection of outliers – Q-test graphing – the least squares principle – linear regression of data.

### **PRACTICALS (FOR INTERNAL ASSESSMENT ONLY):**

1. Calibration of pipette, burette and standard flask
2. Inter-calibration of pipette and standard flask
3. Preparation of primary and secondary standard solutions.
4. Illustration of rejection of outlying data.
5. Illustration of drawing linear regression line (line of best fit).

### **SCHEME OF EXAMINATION:**

|                               |       |  |
|-------------------------------|-------|--|
| External Theory Examination   | ----- | <b>40 marks</b> (to be conducted by University with time duration of 2 Hrs.)   |
| Internal Practical Assessment | ----- | <b>10 marks</b> (to be provided by the teacher as CIA, based on the performance of students in acquiring the above skills) |

### **Reference Books:**

- R. Gopalan and others, Elements of Analytical Chemistry, Sultan chand & Co.
- Dr. Alka Gupta, Analytical Chemistry, Pragati Prakashan
- Willard, H.H., Merritt, L.L., Dean, J. & Settoe, F.A. Instrumental Methods of Analysis. 7<sup>th</sup> Ed. Wadsworth Publishing Co. Ltd., Belmont, California, USA, 1988.
- Skoog, D.A.; West, D.M. & Holler, F.J. Fundamentals of Analytical Chemistry 6<sup>th</sup> Ed., Saunders College Publishing, Fort Worth (1992).
- Harris, D. C. Quantitative Chemical Analysis, W. H. Freeman.
- Dean, J. A. Analytical Chemistry Notebook, McGraw Hill.
- Day, R. A. & Underwood, A. L. Quantitative Analysis, Prentice Hall of India.
- Vogel, A. I. Vogel's Quantitative Chemical Analysis 6<sup>th</sup> Ed., Prentice Hall.

## II – Year – Semester - III

### SEC-1:UCHM237: CHEMICAL TECHNOLOGY & SOCIETY

(30 Lectures)

1-1-0-2

#### **Chemical Technology:**

Basic principles of distillation, solvent extraction, solid-liquid leaching and liquid-liquid extraction, separation by absorption and adsorption. An introduction into the scope of different types of equipment needed in chemical technology, including reactors, distillation columns, extruders, pumps, mills, emulgators. Scaling up operations in chemical industry. Introduction to clean technology.

Chemistry in Nanotechnology Breakthroughs, Chemistry in Computing, Chemistry in Transportation, and Chemistry in the Space Age.

Policies to Enable Innovations in Technology – updating primary chemicals management law to adapt to scientific advancements and to promote that “chemical products are safe for intended use”, while also encouraging innovation.

#### **Society:**

Exploration of societal and technological issues from a chemical perspective. Chemical and scientific literacy as a means to better understand topics like air and water (and the trace materials found in them that are referred to as pollutants); energy from natural sources (i.e. solar and renewable forms), from fossil fuels and from nuclear fission; materials like plastics and polymers and their natural analogues, proteins and nucleic acids, and molecular reactivity and interconversions from simple examples like combustion to complex instances like genetic engineering and the manufacture of drugs.

The innovative products of chemistry lead to cutting edge advancements - applied technology in medical devices, aerospace, computing, cars, fuels etc. - technological advancements that drive innovation, create jobs and enhance safety in our everyday lives.

Communicating costs and benefits of the chemical industry and chemical technology to society – Risk communication.

## **PRACTICALS (FOR INTERNAL ASSESSMENT ONLY):**

1. Determination of Total Suspended Particulates (TSPs) in ambient air.
2. Medicinal compounds extraction using solvent extraction, solid-liquid leaching and liquid-liquid extraction.
3. Adulteration checking in food items.

## **SCHEME OF EXAMINATION:**

|                               |       |  |
|-------------------------------|-------|--|
| External Theory Examination   | ----- | <b>40 marks</b> (to be conducted by University with time duration of 2 Hrs.)   |
| Internal Practical Assessment | ----- | <b>10 marks</b> (to be provided by the teacher as CIA, based on the performance of students in acquiring the above skills) |

## **References:**

- John W. Hill, Terry W. McCreary & Doris K. Kolb, Chemistry for changing times 13<sup>th</sup> Ed.
- <https://www.acs.org/content/acs/en/education.html>



## II Year - Semester - IV

### DSC-1D- UCHM 241: Physical Chemistry-II

(60 Lectures)

3-1-0-3

#### Objective:

- To Study the Electrochemistry
- To Study the Elementary Quantum Mechanics
- To Study the molecular spectroscopic methods: microwave, IR, Raman and electronic spectroscopy.
- To Study the physical properties and molecular structure.

#### UNIT-I ELECTROCHEMISTRY-I

(12 Hours)

Electrical transport-conduction in metals and in electrolyte solutions; specific conductance; equivalent conductance; measurement of equivalent conductance; variation of equivalent conductance with dilution; migration of ions and Kohlrausch law; Ostwald dilution law-uses and limitations; Debye-Huckel-Onsager equation for strong electrolytes (derivation not required).

Transport number; determination by Hittorf method and moving boundary method; determination of degree of dissociation; determination of  $K_a$  of acids; determination of solubility product of sparingly soluble salts; conductometric titrations.

#### UNIT-II ELECTROCHEMISTRY-II

(12 Hours)

Types of reversible electrodes- Gas-metal ion, metal-metal ion, metal-insoluble salt and redox electrodes. Electrode reactions; Nernst equation; derivation of cell E.M.F and single electrode potential; sign conventions; electrochemical series and its significance.

Reversible and irreversible cells; conventional representation of electrochemical cells; E.M.F of cell and its measurements; computation of cell E.M.F.; calculation of thermodynamic quantities of cell reactions ( $\Delta G$ ,  $\Delta H$  and  $\Delta K$ ); concentration cells with and without transport; liquid junction potential; applications of concentration cells.

Definition of pH and  $pK_a$ ; determination of pH by using hydrogen, quinhydrone and glass electrodes by potentiometric method; potentiometric titrations.

Buffers; mechanism of buffer action; Hendersen-Hazel equation; hydrolysis of salts.

### **UNIT-III ELEMENTARY QUANTUM MECHANICS (12 Hours)**

Black body radiation; Plank's radiation law; photoelectric effect; Compton effect; De Broglie hypothesis; Heisenberg's uncertainty principle; Sinusoidal wave equation; Radial and angular wave functions; Probability distribution curves; Hamiltonian operator; Schrodinger wave equation and its significance; physical interpretation of wave function; postulates of quantum mechanics; particle in one dimensional box.

### **UNIT-IV MOLECULAR SPECTROSCOPY-I (12 Hours)**

#### **(a) MICROWAVE SPECTROSCOPY**

Electromagnetic radiation; Regions of the spectrum; Diatomic molecules; selection rules; energy levels of rigid rotor (semi-classical principles); spectral intensity; distribution using population distribution (Maxwell-Boltzmann distribution); determination of bond length; isotope effect.

#### **(b) INFRARED SPECTROSCOPY**

Infrared spectrum; selection rules; energy levels of simple harmonic oscillator; pure vibrational spectrum; intensity; force constant and its determination; qualitative relation between force constant and bond energy; effect of anharmonic motion and isotope on the infrared frequency; vibrational frequencies of different functional groups.

### **UNIT-V MOLECULAR SPECTROSCOPY-II (12 Hours)**

#### **(a) RAMAN SPECTROSCOPY**

Concept of polarisability; selection rules; pure rotational and pure vibrational Raman spectra of diatomic molecules; classical theory of rotational and vibrational Raman spectroscopy, complementarities of Raman and IR spectroscopy, mutual exclusion principle, polarized and depolarized Raman lines.

#### **(b) ELECTRONIC SPECTROSCOPY**

Concept of potential energy curves for bonding and antibonding molecular orbitals; qualitative description of selection rules; Frank-Condon principle; predissociation; qualitative description of  $\sigma$ ,  $\pi$  and  $n$  molecular orbitals and their energy levels; types of electronic transitions.

#### **(c) PHYSICAL PROPERTIES AND MOLECULAR STRUCTURE**

Optical activity and polarization (Clausius-Mossotti equation); dipole moment; induced dipole moment; measurement of dipole moment – temperature and refractivity methods;

dipole moment and structure of molecules. Magnetic properties-paramagnetism, diamagnetism and ferromagnetism.

### **Text Books**

1. Principles of Physical Chemistry - B.R. Puri and Sharma - Shobanlal Nagin Chand & Co.,
2. P.L. Soni, O.P. Dharmarha and U.N. Dash, Textbook of Physical Chemistry, 23rd Edition, Sultan Chand & Sons, New Delhi, 2011.
3. Physical Chemistry - Negi and Anand – Eastern Wiley Pvt.Ltd..
4. Physical Chemistry - Kundu and Jain - S. Chand & Co.
5. Physical Chemistry - K.L Kapoor - Macmillan - 4 volumes
6. Elements of Physical Chemistry - Glasstone and Lewis - Macmillan.
7. C.N. Banwell and E.M. McCash, Fundamentals of Molecular Spectroscopy, 4th Edition, McGraw–Hill Publishing Company Limited, New Delhi, 2002.
8. Gurudeep R. Chatwal and Sham K. Anand, Spectroscopy: Atomic and Molecular, 5th Edition, Himalaya Publishing House, New Delhi, 2013.

### **Reference Books:**

1. Text book of Physical Chemistry - S. Glasstone- Macmillan (India) Ltd.
2. S. Glasstone, *An Introduction to Electrochemistry*, East-West Press Pvt. Ltd., New Delhi, 2007.
3. Fundamentals of Physical Chemistry - Maron and Landor - Colier - Macmillan.
4. Physical Chemistry - G.W. Castellan - Narosa publishing house.
5. Physical Chemistry - Walter J. Moore - Orient Longman.
6. Elements of Analytical Chemistry - R. Gopalan, P.S. Subramanian, K. Rengarajan - S. Chand and sons (1997).
7. Principles of Instrumental Methods of Analysis - D.A Skoog and Saunders - College publications - III edition (1985).
8. Instrumental Methods of Chemical Analysis – B.K. Sharma - Goel Publications.

## II Year - Semester - IV

### DSC-2D: UCHM 242: Organic Chemistry – I

(60 Lectures)

4-1-0-4

#### Objective:

- To Study about the Alkyl and Aryl Halides
- To Study about the Alcohols and Phenols
- To Study about the Carbonyl Compounds
- To Study about the Organic Compounds of Nitrogen
- To Study about the Heterocyclics

#### Unit-I: Alkyl and Aryl Halides

(12Hrs)

**Alkyl halides:** Preparation from alkenes and alcohols. Reactions - hydrolysis, nitrite & nitro formation, nitrile and isonitrile formation, Williamson's synthesis, Elimination vs Substitution

**Aryl halides:** Preparation of chloro-, bromo- and iodo-benzenes from phenol, Sandmeyer and Gattermann reactions. Reactions of aryl halides: Aromatic nucleophilic substitution (replacement by -OH group and effect of nitro substituent. Benzyne mechanism:  $K(Na)NH_2/NH_3$ ).

Reactivity and relative strength of Carbon-Halogen bond in alkyl, allyl, benzyl, vinyl and aryl halides.

#### Unit-II: Alcohols and Phenols

(12 Hrs)

**Alcohols:** Preparation of primary, secondary and tertiary alcohols using Grignard reagent, ester hydrolysis, reduction of aldehydes, ketones, carboxylic acids and esters. Reactions with sodium, HX (Lucas Test), esterification, oxidation (with PCC, alk.  $KMnO_4$ , acidic dichromate, Con.  $HNO_3$ ). Oxidation of diols - Pinacol-Pinacolone rearrangement.

**Phenols:** Preparation by cumene hydroperoxide method, from diazonium salts. Reactions - Electrophilic substitution - nitration, halogenations and sulphonation. Reier-Tiemann reaction, Gattermann-Koch reaction, Houben- Hoesch condensation, Schotten Baumann reaction. Acidic character of phenol, comparative strength of alcohol and phenol.

#### Unit-III: Carbonyl Compounds

(12 Hrs)

Structural significance of the carbonyl function and nomenclature.

**Aldehydes and ketones:** Formaldehyde, acetaldehyde, acetone and benzaldehyde - preparation from acid chlorides & from nitriles. Reactions: reaction with HCN, ROH,  $NaHSO_3$ , amino derivatives. Iodoform test, aldol condensation, Cannizzaro's reaction, Wittig reaction, Benzoin condensation, Clemmensen Reduction and Wolff Kishner reduction. Meerwein-Ponndorf-Verley reduction.

**Carboxylic acids & their derivatives:** Preparation of formic, acetic and benzoic acids. Reactions: Hell-Volhard-Zelinsky reaction, synthetic applications of diethyl malonate &

ethyl acetoacetate. Preparation of acid chlorides, anhydrides, esters and amides from acids and their interconversion. Reactions: comparative study of the nucleophilicity of acyl derivatives. Reformatsky Reaction, Perkin condensation.

#### **Unit-IV: Organic Compounds of Nitrogen**

**(12 Hrs)**

**Nitro compounds:** Preparation of nitroalkanes and nitroarenes. Reduction of nitrobenzene under various conditions, nitro-acinitro tautomerism.

**Amines (aliphatic and aromatic):** Classification, preparation from alkyl halides, Gabriel-Phthalimide synthesis, Hofmann bromamide reaction. Hofmann and Saytzeff elimination, Carbylamine test, Hinsberg test, with HNO<sub>2</sub>, Schotten-Baumann reaction, Electrophilic substitution in aniline: nitration, bromination and sulphonation.

**Diazonium salts:** Preparation from aromatic amines. Conversion to benzene, phenol and azodyes.

#### **Unit-V: Heterocyclics**

**(12 Hrs)**

Molecular Orbital picture and aromatic characteristics of pyrrole, furan, thiophene and pyridine. Methods of synthesis and chemical reactions with emphasis on the mechanism of electrophilic substitution reaction, mechanism of nucleophilic substitution reactions in pyridine derivatives. Comparison of basicity of pyridine, piperidine and pyrrole. Introduction to condensed five- and six-membered heterocyclics. Preparation and reaction of indole, quinoline and isoquinoline with special reference to Bisler-Napieralski synthesis. Mechanism of electrophilic substitution reactions of indole, quinoline and isoquinoline.

#### **Reference Books:**

- Kotz, J.C., Treichel, P.M. & Townsend, J.R. General Chemistry, Cengage Learning India Pvt. Ltd.: New Delhi (2009).
- Petrucci, R.H. General Chemistry, 5<sup>th</sup> Ed., Macmillan Publishing Co.: New York (1985).
- Morrison, R. T. & Boyd, R. N. Organic Chemistry, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- Finar, I. L. Organic Chemistry (Volume 1), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- Finar, I. L. Organic Chemistry (Volume 2), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- Nelson, D. L. & Cox, M. M. Lehninger's Principles of Biochemistry 7<sup>th</sup> Ed., W. H. Freeman.
- Berg, J.M., Tymoczko, J.L. & Stryer, L. Biochemistry, W.H. Freeman, 2002.
- R.T. Morrison & R.N. Boyd: Organic Chemistry, Prentice Hall.
- Peter Sykes: A Guide Book to Mechanism in Organic Chemistry, Orient Longman.
- ArunBahl and B. S. Bahl: Advanced Organic Chemistry, S. Chand.

## DSC- 4D: UCHM 246: PHYSICAL & ORGANIC CHEMISTRY PRACTICAL

(60 Lectures)

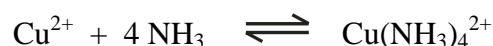
0-1-4-2

### A. PHYSICAL CHEMISTRY

1. Determination of rate constant of acid catalysed hydrolysis of esters at room temperature.
2. Kinetics of persulphate oxidation.
3. Determination of standard potential of  $Zn^{2+}/Zn$ ;  $Cu^{2+}/Cu$ ;  $Ag^+/Ag$  electrodes
4. Determination of the equilibrium constant for the equilibrium



(or)



using amyl alcohol as solvent and methyl red as indicator.

5. Determination of pH using quinhydrone electrode
6. Determination of solubility and solubility product using e.m.f measurement.
7. Estimation of chromate in a solution by spectrophotometry – Verification of Beer-Lambert's Law.

### B. ORGANIC CHEMISTRY:

**Separation of any one of the following mixtures:**

Naphthalene & Benzoic acid

Benzoic acid & Glucose

Naphthalene & Glucose

#### Reference Books:

1. Khosla, B. D.; Garg, V. C. & Gulati, A. Senior Practical Physical Chemistry, R. Chand & Co.: New Delhi (2011).
2. Vogel, A.I., Tatchell, A.R., Furnis, B.S., Hannaford, A.J. and Smith, P.W.G., Vogel's Textbook of Practical Organic Chemistry, Prentice-Hall, 5th edition, 1996.
3. Mann, F.G. & Saunders, B.C. Practical Organic Chemistry Orient-Longman, 1960.
4. Manual of Biochemistry Workshop, 2012, Department of Chemistry, University of Delhi.

**Scheme of Valuation: (Max marks: 50)**

|                                   |       |          |
|-----------------------------------|-------|----------|
| 1. Internal Marks                 | ----- | 10 marks |
| 2. Record (containing both A & B) | ----- | 10 marks |
| 3. Physical Chemistry Experiment  | ----- | 20 marks |
| 4. Organic Separation             | ----- | 10 marks |

### III – Year – Semester -IV

#### SEC-2:UCHM244: ANALYTICAL AND CLINICAL BIOCHEMISTRY

(30 Lectures)

1-1-0-2

#### UNIT-I

(10 Hrs)

##### **Biological Chemistry-I:**

Elementary treatment of digestion and absorption of carbohydrates, proteins and fats:

**Carbohydrates:** Biological importance of carbohydrates, Metabolism, Cellular currency of energy (ATP), Glycolysis, Alcoholic and Lactic acid fermentations, Krebs cycle.

**Proteins:** Aminoacids, peptides and proteins: classification of proteins: Digestion and absorption of proteins, Formation of Urea, Transamination, Deamination, Plasma Protein, Lipotropic factors.

**Lipids:** Definition, Classification, Importance, General Lipid Metabolism, Digestion and Absorption of Fat, Oxidation of Fatty acids, Ketosis, Lipoprotein metabolism classification of lipoprotein, Biological importance of triglycerides and phosphoglycerides and cholesterol.

#### UNIT-2

(10 Hrs)

##### **Biological Chemistry-II:**

**Enzymes:** Elementary treatment of enzymes, cofactors, prosthetic groups and theory of enzyme action. Nomenclature, classification, effect of pH, temperature on enzyme activity, enzyme inhibition.

**Hormones:** Introduction, General Mechanism of actions - Physiological functions of adrenaline, thyroxin, oxytocin, insulin and sex hormones.

Micronutrients and their biological role in human systems. Iron Metabolism - General consideration of Importance of sodium, potassium, calcium, magnesium, chloride and fluoride - Vitamins: General consideration, clinical importance. Definition of Health, WHO standard - Balanced diet.

#### UNIT-3

##### **Biochemical Analysis:**

(10 Hrs)

Principle of estimation and diagnostic approach by blood and urine analysis:

**Blood:** Composition, grouping and Rh factor - collection and preservation of samples. Anaemia, Regulation, estimation and interpretation of data for blood sugar, urea, creatinine, cholesterol and bilirubin. significance of HDL and LDL - Important lipid profile tests.

**Urine:** Collection and preservation of samples, Formation of urine, Composition and estimation of constituents of normal and pathological urine.

Normal and abnormal values of clinical chemistry in relation to human diseases – General consideration and interpretations.



### **PRACTICALS / FIELD VISIT (FOR INTERNAL ASSESSMENT ONLY):**

Students to be taken in small groups to a nearby hospital or clinical laboratory in order to gain a first-hand practical knowledge of the tests they study in this paper and submit a report.

### **SCHEME OF EXAMINATION:**

|                               |       |  |
|-------------------------------|-------|--|
| External Theory Examination   | ----- | <b>40 marks</b> (to be conducted by University with time duration of 2 Hrs.)                               |
| Internal Practical Assessment | ----- | <b>10 marks</b> (to be provided by the teacher as CIA, based on the above report submitted by the student) |

### **Reference Books:**

- T.G. Cooper: Tool of Biochemistry.
- Keith Wilson and John Walker: Practical Biochemistry.
- Alan H Gowenlock: Varley's Practical Clinical Biochemistry.
- Thomas M. Devlin: Textbook of Biochemistry.
- Berg, J.M., Tymoczko, J.L. & Stryer, L. Biochemistry, W.H. Freeman, 2002.
- Talwar, G.P. & Srivastava, M. Textbook of Biochemistry and Human Biology, 3<sup>rd</sup> Ed. PHI Learning.
- Nelson, D. L. & Cox, M. M. Lehninger's Principles of Biochemistry 7<sup>th</sup> Ed.,  
W. H. Freeman.
- Mikes, O. Laboratory Hand Book of Chromatographic & Allied Methods, Elles Harwood Series on Analytical Chemistry, John Wiley & Sons, 1979.

## II – Year – Semester – IV

### SEC-2:UCHM245: CHEMOINFORMATICS

(30 Lectures)

1-1-0-2

**Introduction to Chemo informatics:** History and evolution of chemoinformatics, Use of chemoinformatics, Prospects of chemoinformatics, Molecular Modelling and Structure elucidation.

**Representation of molecules and chemical reactions:** Nomenclature, Different types of notations, SMILES coding, Matrix representations, Structure of Molfiles and Sdfiles, Libraries and toolkits, Different electronic effects, Reaction classification.

**Searching chemical structures:** Full structure search, sub-structure search, basic ideas, similarity search, three dimensional search methods, basics of computation of physical and chemical data and structure descriptors, data visualization.

**Applications:** Prediction of Properties of Compounds; Linear Free Energy Relations; Quantitative Structure-Property Relations; Descriptor Analysis; Model Building; Modeling Toxicity; Structure-Spectra correlations; Prediction of NMR, IR and Mass spectra; Computer Assisted Structure elucidations; Computer Assisted Synthesis Design, Introduction to drug design; Target Identification and Validation; Lead Finding and Optimization; Analysis of HTS data; Virtual Screening; Design of Combinatorial Libraries; Ligand-Based and Structure Based Drug design; Application of Chemoinformatics in Drug Design.

### **PRACTICALS (FOR INTERNAL ASSESSMENT ONLY):**

1. SMILES coding, Matrix representations, Structure of Molfiles and Sdfiles for simple organic molecules
2. Full structure search, sub-structure search, basic ideas, similarity search, three dimensional search methods, basics of computation of physical and chemical data and structure descriptors, data visualization of simple molecules.
3. Prediction of NMR, IR and Mass spectra of simple compounds
4. Ligand-Based and Structure-Based Drug design: Understanding medicinal properties of commercially available drugs.

### **SCHEME OF EXAMINATION:**

|                               |       |  |
|-------------------------------|-------|--|
| External Theory Examination   | ----- | <b>40 marks</b> (to be conducted by University with time duration of 2 Hrs.)   |
| Internal Practical Assessment | ----- | <b>10 marks</b> (to be provided by the teacher as CIA, based on the performance of students in acquiring the above skills) |

### **Hands-on Exercises Reference Books:**

- Andrew R. Leach & Valerie, J. Gillet (2007) An introduction to Chemoinformatics. Springer: The Netherlands.
- Gasteiger, J. & Engel, T. (2003) Chemoinformatics: A text-book. Wiley-VCH.
- Gupta, S. P. (2011) QSAR & Molecular Modeling. Anamaya Pub.: New Delhi.

## II – Year – Semester - IV

### SEC-2:UCHM247: BUSINESS SKILLS FOR CHEMISTS

(30 Lectures)

1-1-0-2

**Chemical knowledge/ skills:** Safe handling of chemical materials, Skills with chemical instrumentation.

**Generic skills:** Planning and design of experiments, Report writing skills, Oral presentation skills, Information retrieval skills

**Problem solving skills:** Team working skills, Time management and organisational skills, Independent learning ability required for continuing professional development

**Business Basics:**

**Key business concepts:** Business plans, market need, project management and routes to market.

Chemistry in Industry

Current challenges and opportunities for the chemistry-using industries, role of chemistry in India and global economies.

**Making money:** Financial aspects of business with case studies

**Intellectual property:** Concept of intellectual property, patents.

### **PRACTICALS / CASE STUDY (FOR INTERNAL ASSESSMENT ONLY):**

1. SWOT analysis of any chemical industry
2. Finance Case Study for a industry
3. How to Set up a Site Visit: Taking suitable example
4. How to prepare a Business Plan: Taking suitable example

(Department of Chemistry can take help of BBA/MBA dept for this course)

### **SCHEME OF EXAMINATION:**

|                               |       |  |
|-------------------------------|-------|--|
| External Theory Examination   | ----- | <b>40 marks</b> (to be conducted by University with time duration of 2 Hrs.)   |
| Internal Practical Assessment | ----- | <b>10 marks</b> (to be provided by the teacher as CIA, based on the performance of students in any one of the above listed activities) |

### **Reference:**

- [www.rsc.org](http://www.rsc.org)
- <http://www.rsc.org/learn-chemistry/resources/business-skills-for-chemists>
- <http://www.rsc.org/learn-chemistry/resources/business-skills-and-commercial-awareness-for-chemists>
- <http://www.rsc.org/learn-chemistry/resources/business-skills-for-chemists/Tutors/ITBC/downloads.php>

**Choice Based Credit System**  
**Syllabus for III B. Sc., (Chemistry) – 5<sup>th</sup> & 6<sup>th</sup> Semesters**  
**(REVISED)**

**IMPORTANT NOTE FOR FIFTH & SIXTH SEMESTERS:**

**1. PRACTICAL EXAMS:**

DSC practical exam and any one DSE practical exam are to be conducted in two continuous sessions of 3 Hrs each on the same day. For the other DSE practical exam, a separate session of 3 hours shall be allotted on another day.

One external and one internal examiner shall be conducting the External University Practical examinations (refer below) and the Internal CIA marks are to be provided by the faculty handling those papers.

| Course          | Internal CIA marks | External Exam marks | Total |
|-----------------|--------------------|---------------------|-------|
| DSC Practical   | 10                 | 40                  | 50    |
| DSE-1 Practical | 5                  | 20                  | 25    |
| DSE-2 Practical | 5                  | 20                  | 25    |

2. FOR DSE THEORY PAPERS, out of 75 marks allotted, 15 marks are for CIA and 60 marks for University written exam.

3. FOR ONE SEC PAPER, the scheme of examination is similar to the one followed for II Year SEC papers as given below:

**SCHEME OF EXAMINATION FOR SEC PAPER:**

External Theory Examination ----- 40 marks (to be conducted by University with time duration of 2 Hrs.)

Internal Practical Assessment ----- 10 marks (to be provided by the teacher as CIA, based on the performance of the student during practical classes – no separate practical examination)

4. GE PAPERS: Of the two GE papers suggested every semester, any one can be offered to the students of other departments, carrying 75% marks for external written exam and 25% marks for internal CIA.

### III - Year – Semester - V

#### DSC - 1E: UCHM 351: INORGANIC CHEMISTRY-II

(60 Hrs)

3-1-0-3

#### Objective:

- To Study the Chemistry of d-block elements
- To Study the Lanthanides and Actinides
- To Study the basics of Co-ordination Compounds and applications
- To Study the theories of coordination compounds and their applications

#### UNIT-I: Chemistry of d-block elements - First transition series (12 Hrs)

General characteristics of d-block elements. Properties of the elements of the first transition series. Relative stabilities of their oxidation states. Extraction from ores and refining of Ti, Mn, Cr, Fe, Co, Ni, Cu and Zn and their uses.

#### UNIT-II: Chemistry of d-block elements –II and III transition series (12 Hrs)

General characteristics – Comparative treatment with their *3d* analogues in respect of ionic radii, oxidation states, magnetic behavior. Metallurgy of silver, gold, platinum and palladium.

#### UNIT III: Lanthanides and Actinides (12Hrs)

(a) Lanthanides: Position of lanthanides in the periodic table. General characteristics of lanthanides. Occurrence, electronic configuration, oxidation states, atomic & ionic radii, lanthanide contraction – causes & consequences, colour, magnetic properties & complex formation. Extraction of lanthanides from monazite sand & separation of lanthanide elements by ion exchange method. Uses of lanthanides and their compounds.

(b) Actinides: Position of actinides in the periodic table. General characteristics of actinides: occurrence, electronic configuration, oxidation states, ionic radii of tripositive and tetrapositive cations, colour of  $M^{3+}$  and  $M^{4+}$  cations, magnetic properties and complex formation. Comparison between lanthanides and actinides. Th and U (extraction only). Separation of Np, Pu and Am from U.

#### UNIT IV: Co-ordination compounds-I: (12 Hrs)

Definition of terms used - classification of ligands - chelation and effect of chelation - Co-ordination number and stereo chemistry of complexes –Werner's theory - EAN rule - Nomenclature of mono nuclear and binuclear (bridged) complexes. Isomerism in complexes – ionization isomerism, hydrate isomerism, linkage isomerism, ligand isomerism, co-ordination isomerism, polymerization isomerism, geometrical and optical isomerism in 4 and 6 co-ordinated complexes.

Applications of Co-ordination compounds in qualitative and quantitative analysis - Applications in industry and medicine.

**UNIT V: Co-ordination compounds-II:**

**(12 Hrs)**

Valence bond theory - hybridisation - geometry and magnetic properties - limitations of VBT. Crystal field theory - splitting of *d*-orbitals in octahedral, tetrahedral and square planar complexes - crystal field stabilisation energy - calculation of CFSE in tetrahedral and octahedral complexes - Low spin and high spin complexes – explanation of magnetic properties, colour and geometry using CFT - Comparison of VBT and CFT.

Basic principles of molecular orbital theory (MOT) of co-ordination compounds as applied to octahedral complexes without  $\pi$ -bonding and its MO correlation diagram of  $[\text{Co}(\text{NH}_3)_6]^{3+}$ - The adjusted crystal field theory (ACFT) or the ligand field theory (LFT) - Types of magnetic behavior. Methods of determination of magnetic susceptibility and magnetic moments (Guoy's method only). The electronic spectrum of  $[\text{Ti}(\text{H}_2\text{O})_6]^{3+}$  ion in solution. Spectrochemical series.

**Reference Books:**

- Cotton, F.A., Wilkinson, G. & Gaus, P.L. Basic Inorganic Chemistry, 3<sup>rd</sup> Ed., Wiley.
- Douglas, B.E., McDaniel, D.H. & Alexander, J.J. Concepts and Models in Inorganic Chemistry, John Wiley & Sons.
- Huheey, J.E., Keiter, E.A., Keiter, R.L. & Medhi, O.K. Inorganic Chemistry: Principles of Structure and Reactivity, Pearson Education India, 2006.
- Rodgers, G.E. Inorganic & Solid State Chemistry, Cengage Learning India Ltd., 2008. Miessler, G. L. & Donald, A. Tarr. Inorganic Chemistry 4<sup>th</sup> Ed., Pearson, 2010.
- Atkin, P. Shriver & Atkins' Inorganic Chemistry 5<sup>th</sup> Ed. Oxford University Press (2010)



### III Year – Semester - V

#### CHEMISTRY-DSE (ELECTIVES)

#### DSE: UCHM 352: APPLICATIONS OF COMPUTERS IN CHEMISTRY

(60 Hrs)

4-1-0-4

#### Objective:

- To know the basics of computer science
- To learn some basic languages of computer science.
- To study some numerical methods
- To learn handling of experimental data and control structures
- To know some important applications in chemistry

:

#### Unit-I

##### Basics:

(12 Hrs)

Constants, variables, bits, bytes, binary and ASCII formats, arithmetic expressions, hierarchy of operations, inbuilt functions. Basic computer organization, processor and memory – main memory, secondary storage devices and storage hierarchy. Software – relationship between hardware and software – types of software. Planning the computer program – algorithm and flowcharts. Basics of operating systems.

#### Unit-II

##### Languages:

(12 Hrs)

Compiled versus interpreted languages. Debugging. Simple programs using these concepts. Computer languages – machine language, assembly language, assembler, compiler, interpreter and programming languages –  
Elements of the BASIC language. BASIC keywords and commands. Logical and relative operators. Strings and graphics.  
C language – introduction, C compiler, operating systems and preprocessor directives - variables, constants, operators, input and output functions.

#### Unit-III

##### Numerical methods:

(12 Hrs)

*Roots of equations:* Numerical methods for roots of equations: Quadratic formula, iterative method, Newton-Raphson method, Binary bisection and Regula-Falsi.

*Differential calculus:* Numerical differentiation.

*Integral calculus:* Numerical integration (Trapezoidal and Simpson's rule), probability distributions and mean values.

#### Unit-IV

(12 Hrs)

Simultaneous equations: Matrix manipulation: addition, multiplication. Gauss-Seidel method. Interpolation, extrapolation and curve fitting: Handling of experimental data.

Control structures – conditional, looping, goto, break, switch and continue statements, functions, arrays and pointers.

#### Unit-V

##### Applications in Chemistry:

(12 Hrs)

Calculation of the radius of the first Bohr orbit for an electron, Calculation of electronegativity of an element using Pauling's relation. Calculation of empirical formulae of hydro carbon, calculation of reduced mass of a few diatomic molecules, determination of the wave numbers of spectral lines of hydrogen atom.

Conceptual background of molecular modelling: Potential energy surfaces. Elementary ideas of molecular mechanics and practical MO methods.

#### Reference Books:

1. Harris, D. C. *Quantitative Chemical Analysis*. 6<sup>th</sup> Ed., Freeman (2007) Chapters 3-5.
2. Levier. de, *How to use Excel in analytical chemistry and in general scientific data analysis*, Cambridge Univ. Press (2001) 487 pages.
3. Noggle, J. H. *Physical chemistry on a Microcomputer*. Little Brown & Co. (1985).
4. Venit, S.M. *Programming in BASIC: Problem solving with structure and style*. Jaico Publishing House: Delhi (1996).
5. McQuarrie, D. A. *Mathematics for Physical Chemistry*, University Science Books (2008).
6. Mortimer, R. *Mathematics for Physical Chemistry*, 3<sup>rd</sup> Ed. Elsevier (2005).
7. Steiner, E. *The Chemical Maths Book*, Oxford University Press (1996).
8. Yates, P. *Chemical Calculations*. 2<sup>nd</sup> Ed. CRC Press (2007).

## DSE: UCHM 352: APPLICATIONS OF COMPUTERS IN CHEMISTRY-PRACTICAL

(30 Lectures)

0-1-4-2

### Computer programs based on numerical methods for

1. Roots of equations: (e.g. volume of van der Waals gas and comparison with ideal gas, pH of a weak acid).
2. Numerical differentiation (e.g., change in pressure for small change in volume of a van der Waals gas, potentiometric titrations).
3. Numerical integration (e.g. entropy/ enthalpy change from heat capacity data), probability distributions (gas kinetic theory) and mean values.
4. Matrix operations. Application of Gauss-Siedel method in colourimetry.
5. Computer Lab based instruction on the use of computer and internet in learning.
6. Use of educational softwares, information mining from internet and using INFLIBNET/NICNET, NPTEL and VIRTUAL LABS OF MHRD.
7. Use of Spread sheets in Data handling and presentation.
8. Introduction to chemical structure drawing, visualization of molecules using chemistry softwares.

### Reference Books:

- McQuarrie, D. A. Mathematics for Physical Chemistry University Science Books (2008).
- Mortimer, R. Mathematics for Physical Chemistry. 3<sup>rd</sup>Ed. Elsevier (2005).
- Steiner, E. The Chemical Maths Book Oxford University Press (1996).
- Yates, P. Chemical Calculations. 2<sup>nd</sup> Ed. CRC Press (2007).
- Harris, D. C. Quantitative Chemical Analysis. 6<sup>th</sup> Ed., Freeman (2007) Chapters 3-5.
- Levie, R. de, How to use Excel in analytical chemistry and in general scientific data analysis, Cambridge Univ. Press (2001) 487 pages.
- Noggle, J. H. Physical Chemistry on a Microcomputer. Little Brown & Co. (1985).
- Venit,S.M. Programming in BASIC: Problem solving with structure and style. JaicoPublishing House: Delhi (1996).

### Scheme of Valuation: (Max marks: 25)

|   |       |          |
|---|-------|----------|
| 1. Internal Marks                       | ----- | 5 marks  |
| 2. Record                               | ----- | 5 marks  |
| 3. Viva                                 | ----- | 5 marks  |
| 4. Any one activity from the above list | ----- | 10 marks |

## DSE: UCHM 353: ANALYTICAL METHODS IN CHEMISTRY

(60 Hrs)

4-1-0-4

### Objective:

- To Study the gravimetric method of analysis
- To Study the colorimetric method
- To Study the radiochemical and thermo analytical method
- To learn Polarography and solvent extraction methods
- To learn Chromatographic methods

### UNIT-I GRAVIMETRIC METHOD

(12 Hrs)

Principles of gravimetric analysis – Gravimetric factor – calculations involved – Conditions for precipitation – Theory of precipitation – Types of precipitants - organic precipitants & advantages – Purity of precipitates – Co-precipitation and post-precipitation – Precipitation from homogeneous solution; Crucibles – types and maintenance – washing of the precipitates – Drying and ignition of precipitates.

### UNIT-II COLORIMETRIC METHOD

(12 Hrs)

Quantitative aspects of absorption of radiation – Beer-Lambert's Law – derivation of equation – deviation from Beer-Lambert's Law – Methods of doing Colorimetric Analysis – Standard series method, colorimetric titration, Duboscq colorimeter, Photo electric colorimeter and Spectrophotometric method – instrumentation, single beam and double beam instruments, construction of calibration plots for quantitative analysis – Applications of colorimetry : Molar composition of complexes by Job's method and mole ratio method – Determination of Iron and Manganese compounds – Simultaneous determination of metal ions (Cr and Mn).

### UNIT-III RADIO CHEMICAL AND THERMO ANALYTICAL METHODS (12 Hrs)

#### Radiochemical Methods

Properties of radioisotopes – Isotopic tracing – Isotopic dilution analysis – Neutron activation analysis – Limitations of radioanalytical methods.

#### Thermo analytical methods:

Principles of TGA and DTA – Honda's Balance – Outlines of Instrumentation (block diagrams only) – Application in  $\text{CaC}_2\text{O}_4 \cdot \text{H}_2\text{O}$  and  $(\text{CH}_3\text{COO})_2\text{Ca} \cdot \text{H}_2\text{O}$  – factors affecting TGA & DTA curves.

Thermometric titration – Principle and instrumentation of thermometric titration and its application using HCl (vs) NaOH.

## **UNIT-IV POLAROGRAPHY AND SOLVENT EXTRACTION METHODS (12 Hrs)**

### **(a) Polarography**

Basic principles – DME – migration, residual, limiting and diffusion currents- Use of supporting electrolytes-advantages and disadvantages –The Ilkovic equation (derivation not required) and significance- experimental assembly- current voltage curve- oxygen wave-influence of temperature and agitation on diffusion layer. Half wave potential ( $E_{1/2}$ )– Experimental set up – Applications – Polarography as an analytical tool in quantitative and qualitative analysis - Determination of copper and zinc in brass.

### **(b) Solvent Extraction:**

Principles- techniques of solvent extraction – Batch extraction, continuous extraction – continuous extraction of liquids and solids – Soxhlet extraction – counter-current extraction – Factors favouring solvent extraction of inorganic species – Application of Solvent extraction.

## **UNIT-V CHROMATOGRAPHIC METHODS : (12 Hrs)**

Theory and principles – Classification of chromatographic methods -

- (a) Column Chromatography: Principles and experimental procedures – Adsorbents and Solvent systems – Applications.
- (b) Thin layer chromatography: Principles and experimental procedures – Adsorbents – preparation of TLC plates –  $R_f$  values - Applications – Separation of dyes.
- (c) Paper Chromatography: Principles – ascending, descending and radial techniques –  $R_f$  values – Applications – Separation of Amino acids.
- (d) Gas liquid chromatography: Principles – Instrumentation – Types of Columns – Types of Detectors – Applications.

### **Text Books:**

1. Elements of analytical chemistry by Gopalan R & Subramanian, Sultan chand & Co.
2. Analytical chemistry by Dr. Alka Gupta, Pragati Prakashan

### **Reference Books:**

- Jeffery, G.H., Bassett, J., Mendham, J. & Denney, R.C. Vogel's Textbook of Quantitative Chemical Analysis, John Wiley & Sons, 1989.
- Willard, H.H., Merritt, L.L., Dean, J.A. and Settle, F. A., Instrumental Methods of Analysis, CBS Publishers, 7th Edition, 1988.
- Christian, G.D; Analytical Chemistry, 6th Ed. John Wiley & Sons, New York, 2004.
- Harris, D. C. Exploring Chemical Analysis, Ed. New York, W.H. Freeman, 2001.
- Khopkar, S.M. Basic Concepts of Analytical Chemistry. New Age, International Publisher, 2009.
- Skoog, D.A, Holler, S.J., Nilman, T.A., Principles of Instrumental Analysis, Cengage Learning India Ed. (Skoog, D.A, Holler, S.J., Nilman, T.A., Principles of Instrumental Analysis, 5th Edn., Saunders college publishing, London, 1998.)

- Mikes, O. Laboratory Hand Book of Chromatographic & Allied Methods, Elles Harwood Series on Analytical Chemistry, John Wiley & Sons, 1979.
- Ditts, R.V. Analytical Chemistry; Methods of Separation, van Nostrand, 1974.
- Ewing, G.W., Instrumental Methods of Chemical Analysis, 5th Edition, McGraw-Hill, New York, 1988.

**DSE: UCHM 353: ANALYTICAL METHODS IN CHEMISTRY-PRACTICAL**

**(30 Hrs)**

**0-1-4-2**

**Any EIGHT experiments from the list given below:**

1. Paper chromatographic separation of  $\text{Fe}^{3+}$ ,  $\text{Al}^{3+}$ , and  $\text{Cr}^{3+}$ .
2. Paper chromatographic separation of  $\text{Ni}^{2+}$ ,  $\text{Co}^{2+}$ ,  $\text{Mn}^{2+}$  and  $\text{Zn}^{2+}$
3. Separation and identification of the monosaccharides present in the given mixture (glucose & fructose) by paper chromatography. Reporting the  $R_f$  values.
4. Separate a mixture of Sudan yellow and Sudan Red by TLC technique and identify them on the basis of their  $R_f$  values.
5. Chromatographic separation of the active ingredients of plants, flowers and juices by TLC
6. To separate a mixture of  $\text{Ni}^{2+}$  &  $\text{Fe}^{2+}$  by complexation with DMG and extracting the  $\text{Ni}^{2+}$ -DMG complex in chloroform.
7. Solvent extraction of zirconium with amberliti LA-1, separation from a mixture of irons and gallium.
8. Determination of  $pK_a$  values of indicator by colorimetry.
9. Colorimetric determination of Manganese.
10. Determine the composition of the ferric-salicylate/ ferric-thiocyanate complex by Job's method.

**Scheme of Valuation: (Max marks: 25)**

|   |       |          |
|---|-------|----------|
| 5. Internal Marks                         | ----- | 5 marks  |
| 6. Record                                 | ----- | 5 marks  |
| 7. Viva                                   | ----- | 5 marks  |
| 8. Any one experiment from the above list | ----- | 10 marks |

### **Reference Books:**

- Jeffery, G.H., Bassett, J., Mendham, J. & Denney, R.C. Vogel's Textbook of Quantitative Chemical Analysis, John Wiley & Sons, 1989.
- Willard, H.H., Merritt, L.L., Dean, J. & Settoe, F.A. Instrumental Methods of Analysis, 7<sup>th</sup> Ed. Wadsworth Publishing Company Ltd., Belmont, California, USA, 1988.
- Christian, Gary D; Analytical Chemistry, 6<sup>th</sup> Ed. John Wiley & Sons, New York, 2004.
- Harris, Daniel C: Exploring Chemical Analysis, Ed. New York, W.H. Freeman, 2001.
- Khopkar, S.M. Basic Concepts of Analytical Chemistry. New Age, International Publisher, 2009.
- Skoog, D.A. Holler F.J. & Nieman, T.A. Principles of Instrumental Analysis, Cengage Learning India Ed.
- Mikes, O. Laboratory Hand Book of Chromatographic & Allied Methods, Elles Harwood Series on Analytical Chemistry, John Wiley & Sons, 1979.
- Ditts, R.V. Analytical Chemistry; Methods of Separation, van Nostrand, 1974.

## DSE: UCHM 354: NANO CHEMISTRY

(60 Hrs)

4-1-0-4

### Objective:

- To introduce the basics of nanotechnology and nanochemistry.
- To study the synthesis of nano particles
- To learn the preparation, properties and applications of some nano materials and nano architecture
- To learn the instrumental techniques used in characterization of nano materials
- To study carbon nanostructures and their applications.

### UNIT-I BASICS OF NANO CHEMISTRY:

(12 Hrs)

Definition, length scales and importance of nanoscale and its technology – Classification of nanomaterials (0D, 1D and 2D) - self assembly of materials – self-assembled nanostructures – porous solids, nanowires, nanomachines and quantum dots.

### UNIT-II NANO PARTICLES:

(12 Hrs)

Introduction – types of nanoparticles – preparation, properties and uses of gold, silicon, silver, zinc oxide, iron oxide, alumina and titania nanoparticles. Techniques to synthesize nanoparticles – top down and bottom up approaches – common growth methods.

### UNIT-III NANO MATERIALS

(12 Hrs)

Overview of nanostructures and nanomaterials: classification.

Preparation, properties and applications of carbon nanotubes, nanorods, nano fibre and nanoclay – toxic effects of nanomaterials.

Nanoarchitecture - control of nanoarchitecture - one dimensional control.

### UNIT-IV CHARACTERIZATION OF NANO MATERIALS:

(12 Hrs)

Electron microscopes – scanning electron microscopes (SEM) – transmission electron microscopes (TEM) – scanning probe microscopy – atomic force microscopy (AFM) – scanning tunneling electron microscope (STEM) – basic principles only.

### UNIT-V CARBON NANOSTRUCTURES & APPLICATIONS:

(12 Hrs)

Synthesis and purification of carbon nanotubes, Singlewalled carbon nanotubes and multiwalled carbon nanotubes, Structure-property relationships - Fullerenes, carbon nanotubes and graphene.

Applications of nanomaterials in electronics, optics, catalysis, computers, sensors, transportation, medicine and in environment related issues (detailed discussion not required).



**Books for study:**

1. Nanotechnology, S. Shanmugam, MJP Publishers, Chennai. (2010).
2. A Handbook on Nanochemistry, Patrick Salomon, Dominant Publishers and Distributors, New Delhi.
3. Nanobiotechnology, S. Balaji, MJP Publishers, Chennai. (2010).
4. Nano: The Essentials, T. Pradeep, Tata Mc-Graw Hill, New Delhi (2007).
5. The Chemistry of Nanomaterial: Synthesis, Properties and Applications, Vol. I and II, CNR Rao, Springer (2006).
6. Nanotechnology: Basic Science and Emerging Technologies, Mick Wilson, Kamali Kannangara, Geoff Smith, Michelle Simmons, Burkhard Raguse, Overseas Press (2005).
7. Nanochemistry, G. B. Segreev, Elsevier, Science, New York, (2006).

## DSE: UCHM 354: NANO CHEMISTRY -PRACTICAL

(30 Hrs)

0-1-4-2

**Any EIGHT experiments from the list given below:**

**Exploring the nano world:**

1. Synthesis of hydrogel by co-precipitation method.
2. Synthesis of silver and gold metal nanoparticles.
3. Synthesis of Aqueous Ferrofluid Nanoparticles
4. Synthesis of Ruby Red Colloidal Gold Nanoparticles
5. Synthesis of Cholesteryl Ester Liquid Crystals
6. Investigation of a Liquid Crystal Watch
7. Calibration of a Liquid Crystal Mood Ring
8. Make a Liquid Crystal Pixel
9. Graphene preparation from graphite with sticky tape
10. Nitinol wire Train Nitinol to a desired shape.
11. Preparation of Surface Conductive Glass
12. Titanium Dioxide Raspberry Solar Cell

**Reference:**

- Fahlman, B.D. Materials Chemistry, Springer, 2004.
- <http://www.chymist.com/Laboratory%20Experiments.htm>

**Scheme of Valuation: (Max marks: 25)**

- |   |       |          |
|---|-------|----------|
| 1. Internal Marks                         | ----- | 5 marks  |
| 2. Record                                 | ----- | 5 marks  |
| 3. Viva                                   | ----- | 5 marks  |
| 4. Any one experiment from the above list | ----- | 10 marks |

## DSE: UCHM 355: GREEN CHEMISTRY

(60 Hrs)

4-1-0-4

### Objective:

- To introduce the basic principles of green chemistry.
- To study the green solvents and reagents.
- To learn the green catalysis and reactions.
- To learn the green chemistry synthesis of some real world cases
- To understand future trends in green chemistry.

### UNIT-I

#### Introduction to the basic principles of Green Chemistry:

(12 Hrs)

The need for Green Chemistry and its goals. Basic Principles of Green Chemistry -Prevention of Waste, Concept of atom economy, Calculation of atom economy in Rearrangement Reactions, Addition Reactions, Substitution Reactions and elimination Reactions, Prevention or Minimization of Hazardous Products, Designing Safer Chemicals, Energy Requirements for Synthesis, Selection of appropriate Solvent, Selection of Starting Materials, Use of Protecting Groups, Use of Catalyst, Biodegradable Products Design, Designing of Manufacturing Plants, Strengthening of Analytical Techniques.

### UNIT-II

#### Green Solvents and Reagents:

(12 Hrs)

**Green Solvents:** Definition, Reactions in Acidic Ionic Liquids-Friedel-Crafts reaction of Naphthalene, Reactions in Neutral Ionic Liquids-Hydrogenations, Diel's-Alder Reaction, O-Alkylation and N-alkylation, Methylene Insertion Reactions.

**Green Reagents:** Definition, Dimethylcarbonate, Polymer Supported Reagents-Polymer Supported Peracids, Polymer Supported Chromic Acid, Poly-N-Bromosuccinimide (PNBS), Polystyrene Wittig Reagent, Polymeric Phenylthiomethyl Lithium Reagent.

### UNIT-III

#### Green catalysis/reactions:

(12 Hrs)

Green catalysts- Definition, Types of Green catalyst. Catalysis and green chemistry-Comparison of heterogeneous and homogeneous catalysis, biocatalysis, asymmetric catalysis and photocatalysis. Biocatalysis(Microbial and Enzymes)and phase-transfer catalysis.

*Microwave-assisted reaction in water* – Hoffmann elimination, hydrolysis of methyl benzoate to benzoic acid, oxidation of toluene to benzoic acid. *Microwave-assisted reactions in organic solvents* – Esterification, Fries rearrangement, Diels-Alder reactions and decarboxylation reaction. *Ultrasound-assisted reactions* – oxidation, reduction and Simons-Smith Reaction.

## UNIT-IV

### Green synthesis and Some real world cases:

(12 Hrs)

**Green synthesis of the following compounds:** Adipic acid, catechol, disodium iminodiacetate, ibuprofen and paracetamol.

**Green chemistry in some real world cases:** Surfactants for carbon dioxide – replacing smog producing and ozone depleting solvents with CO<sub>2</sub> for precision cleaning and dry cleaning of garments. Designing of Environmentally safe marine antifoulant. Rightfit pigment: synthetic azopigments to replace toxic organic and inorganic pigments. An efficient, green synthesis of a compostable and widely applicable plastic (poly lactic acid) made from corn. Healthier fats and oil by Green Chemistry: Enzymatic interesterification for production of no Trans-Fats and Oils, Development of fully Recyclable Carpet: Cradle to Cradle Carpeting.

## UNIT-V

### Future Trends in Green Chemistry:

(12 Hrs)

Oxidation reagents and catalysts, biomimetic and multifunctional reagents. Combinatorial Green Chemistry. Proliferation of solvent-less reactions. Non-covalent derivatization. Green Chemistry in sustainable development.

### References

1. V. Kumar, *An Introduction to Green Chemistry-for Graduate and Post-graduate students as per new UGC Syllabus*, Vishal Publishing Co., Jaladhar, India
2. Stanley E. Manahan, *Green Chemistry - and the ten commandments of sustainability*, 2 ed., ChemChar Research, Inc., Columbia, MO 65201 U.S.A.
3. Rs. Sanghi and M.M.Srinivatava, *Green Chemistry: Environmental Friendly Alternatives*, Narosa Publishing House, New Delhi.
4. V.K. Ahluwalia, *Green Chemistry*, Narosa, New Delhi (2011).
5. G. L. Willingham and A. H. Jacobson *Designing an Environmentally Safe Marine Antifoulant*, *ACS Symposium Series*, Vol. 640, American Chemical Society, (1996).
6. Michael C Cann; Thomas P Umile, *Real-world cases in green chemistry*, Volume II, American Chemical Society, Washington (2008).
7. M Lancaster, *Green Chemistry, An Introductory Text*- RSC Publishing, 3<sup>rd</sup> Edition (2016).
8. Ryan, M.A. & Tinnesand, M. *Introduction to Green Chemistry*, American Chemical Society, Washington (2002).

## DSE: UCHM 355: GREEN CHEMISTRY-PRACTICAL

(30 Hours)

Any EIGHT experiments from the following types:

1. Safer starting materials

- Preparation and characterization of nanoparticles of gold using tea leaves.

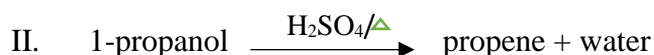
2. Using renewable resources

- Preparation of biodiesel from vegetable/ waste cooking oil.

3. Avoiding waste

Principle of atom economy.

- Use of molecular model kit to stimulate the reaction to investigate how the atom economy can illustrate Green Chemistry.
- Preparation of propene by two methods can be studied
  - I. Triethylamine ion+ OH<sup>-</sup> → propene + trimethyl propene + water



4. Green Methods of Synthesis:

Adipic acid, catechol, disodium iminodiacetate (alternative to Strecker synthesis)

5. Use of enzymes as catalysts

- Benzoin condensation using Thiamine Hydrochloride as a catalyst instead of cyanide.

6. Alternative Green solvents

- Extraction of D-limonene from orange peel using liquid CO<sub>2</sub> prepared from dry ice.
- Mechanochemical solvent free synthesis of azomethines

7. Alternative sources of energy

- Solvent free, microwave assisted one pot synthesis of phthalocyanine complex of copper (II).
- Microwave assisted reactions in water: Hofmann Elimination, methyl benzoate to benzoic acid, oxidation of toluene and alcohols; microwave assisted reactions in organic solvents Diels-Alder reaction and Decarboxylation reaction
- Photo reduction of benzophenone to benzo pinacol in the presence of sunlight.

### Reference Books:

1. Anastas, P.T & Warner, J.C. Green Chemistry: Theory and Practice, Oxford University Press (1998).
2. Kirchoff, M. & Ryan, M.A. Greener approaches to undergraduate chemistry experiment. American Chemical Society, Washington DC (2002).
3. Ryan, M.A. Introduction to Green Chemistry, Tinneland; (Ed), American Chemical Society, Washington DC (2002).
4. Sharma, R.K.; Sidhwani, I.T. & Chaudhari, M.K. I.K. Green Chemistry Experiment: A monograph International Publishing House Pvt Ltd. New Delhi. Bangalore ISBN 978-93-81141-55-7 (2013).
5. Cann, M.C. & Connelly, M. E. Real world cases in Green Chemistry, American Chemical Society (2008).
6. Lancaster, M. Green Chemistry: An Introductory Text RSC Publishing, 2<sup>nd</sup> Edition, 2010.

7. Pavia, D.L., Lampman, G.M., Kriz, G.S. & Engel, R.G. Introduction to Organic Laboratory Techniques: A Microscale and Macro Scale Approach, W.B.Saunders, 1995.

**Scheme of Valuation: (Max marks: 25)**

|   |       |          |
|---|-------|----------|
| 1. Internal Marks                         | ----- | 5 marks  |
| 2. Record                                 | ----- | 5 marks  |
| 3. Viva                                   | ----- | 5 marks  |
| 4. Any one experiment from the above list | ----- | 10 marks |

**DSE: UCHM 356: ORGANOMETALLICS, BIOINORGANIC CHEMISTRY AND  
POLYNUCLEAR HYDROCARBONS**

**(60 Hrs)**

**4-1-0-4**

**Objective:**

- To introduce the chemistry of 3d metals.
- To study the organometallic compounds.
- To learn the Bio-Inorganic chemistry.
- To learn the polynuclear and heteronuclear aromatic compounds
- To study active methylene compounds.

**UNIT-I : Chemistry of 3d metals:**

**(12 Hrs)**

Oxidation states displayed by Cr, Fe, Co, Ni and Co.

A study of the following compounds (including preparation and important properties);

Peroxo compounds of Cr,  $K_2Cr_2O_7$ ,  $KMnO_4$ ,  $K_4[Fe(CN)_6]$ , sodium nitroprusside,  $[Co(NH_3)_6] Cl_3$ ,  $Na_3[Co(NO_2)_6]$ .

**UNIT-II : Organometallic Compounds:**

**(12 Hrs)**

Definition and Classification with appropriate examples based on nature of metal- carbon bond (ionic, s, p and multicentre bonds). Structures of methyl lithium, Zeiss salt and ferrocene. EAN rule as applied to carbonyls. Preparation, structure, bonding and properties of mononuclear and polynuclear carbonyls of 3d metals. p-acceptor behaviour of carbon monoxide. Synergic effects (VB approach)- (MO diagram of CO can be referred to for synergic effect to IR frequencies).

**UNIT-III : Bio-Inorganic Chemistry:**

**(12 Hrs)**

A brief introduction to bio-inorganic chemistry. Role of metal ions present in biological systems with special reference to  $Na^+$ ,  $K^+$  and  $Mg^{2+}$  ions: Na/K pump; Role of  $Mg^{2+}$  ions in energy production and chlorophyll. Role of  $Ca^{2+}$  in blood clotting, stabilization of protein structures and structural role (bones).

**UNIT-IV : Polynuclear and heteronuclear aromatic compounds:**

**(12 Hrs)**

Properties of the following compounds with reference to electrophilic and nucleophilic substitution: Naphthalene, Anthracene, Furan, Pyrrole, Thiophene, and Pyridine.

**UNIT-V : Active methylene compounds:**

**(12 Hrs)**

Preparation: Claisen ester condensation. Keto-enol tautomerism.

Reactions: Synthetic uses of ethylacetoacetate (preparation of non-heteromolecules having upto 6 carbon).

**Reference Books:**

- James E. Huheey, Ellen Keiter & Richard Keiter: Inorganic Chemistry: Principles of Structure and Reactivity, Pearson Publication.
- G.L. Miessler & Donald A. Tarr: Inorganic Chemistry, Pearson Publication.
- J.D. Lee: A New Concise Inorganic Chemistry, E.L.B.S.
- F.A. Cotton & G. Wilkinson: Basic Inorganic Chemistry, John Wiley & Sons.
- I.L. Finar: Organic Chemistry (Vol. I & II), E.L.B.S.
- John R. Dyer: Applications of Absorption Spectroscopy of Organic Compounds, Prentice Hall.
- R.M. Silverstein, G.C. Bassler & T.C. Morrill: Spectroscopic Identification of Organic Compounds, John Wiley & Sons.
- R.T. Morrison & R.N. Boyd: Organic Chemistry, Prentice Hall.
- Peter Sykes: A Guide Book to Mechanism in Organic Chemistry, Orient Longman.
- Arun Bahl and B. S. Bahl: Advanced Organic Chemistry, S. Chand.



**DSE: UCHM 356: ORGANOMETALLICS, BIOINORGANIC CHEMISTRY AND  
POLYNUCLEAR HYDROCARBONS -PRACTICAL**

**(30 Hrs)**

**0-1-4-2**

1. Preparation of any two of the following complexes and measurement of their conductivity:
  - (i) tetra aminecarbonatocobalt (III) nitrate
  - (ii) tetraamminecopper (II) sulphate
  - (iii) potassium trisoxalatoferrate (III) trihydrate
2. Compare the conductance of the complexes with that of M/1000 solution of NaCl, MgCl<sub>2</sub> and LiCl<sub>3</sub>.
3. Preparation of the following:
  1. Ferric alum
  2. Potash alum
  3. Mohr Salt from Kipp's waste
  4. Nickel dimethyl glyoximate
  5. Trithioureacopper (I) sulphate

**Reference Books:**

- A.I. Vogel: Qualitative Inorganic Analysis, Prentice Hall, 7<sup>th</sup> Edn.
- A.I. Vogel: Quantitative Chemical Analysis, Prentice Hall, 6<sup>th</sup> Edn.
- Vogel, A.I., Tatchell, A.R., Furnis, B.S., Hannaford, A.J. & Smith, P.W.G.,  
Textbook of Practical Organic Chemistry, Prentice-Hall, 5<sup>th</sup> edition, 1996.
- Mann, F.G. & Saunders, B.C. Practical Organic Chemistry Orient-Longman, 1960.

**Scheme of Valuation: (Max marks: 25)**

|   |       |          |
|---|-------|----------|
| 1. Internal Marks                         | ----- | 5 marks  |
| 2. Record                                 | ----- | 5 marks  |
| 3. Viva                                   | ----- | 5 marks  |
| 4. Any one experiment from the above list | ----- | 10 marks |

## **DSE: UCHM 357: RESEARCH METHODOLOGY FOR CHEMISTRY**

**(60 Hrs)**

**5-2-0-5**

### **Objective:**

- To introduce the literature survey
- To study the methods of scientific research and writing papers
- To learn how to carryout research in chemistry
- To learn about chemical safety and ethical handling of chemicals
- To learn data handling

### **UNIT-I : Literature Survey:**

**(12 Hrs)**

Print: Sources of information: Primary, secondary, tertiary sources; Journals: Journal abbreviations, abstracts, current titles, reviews, monographs, dictionaries, text-books, current contents, Introduction to Chemical Abstracts and Beilstein, Subject Index, Substance Index, Author Index, Formula Index, and other Indices with examples.

Digital: Web resources, E-journals, Journal access, TOC alerts, Hot articles, Citation index, Impact factor, H-index, E-consortium, UGC infonet, E-books, Internet discussion groups and communities, Blogs, Preprint servers, Search engines, Scirus, Google Scholar, ChemIndustry, Wiki- Databases, ChemSpider, Science Direct, SciFinder, Scopus.

### **UNIT-II : Methods of Scientific Research and Writing Scientific Papers: (12 Hrs)**

Reporting practical and project work. Writing literature surveys and reviews. Organizing a poster display. Giving an oral presentation.

Writing scientific papers – justification for scientific contributions, bibliography, description of methods, conclusions, the need for illustration, style, publications of scientific work. Writing ethics. Avoiding plagiarism.

### **UNIT-III : Research in Chemistry**

**(12 Hrs)**

Selecting a topic – hypothesis- design of experiment: variables, correlation and causality, sampling, use of controls, experimental bias, analysis, results, discussion of results, models., statistical analysis of experimental data using computers, mean, mode, deviation, standard deviation, plotting graph using spread sheet, preparation of seminar papers, project etc. using computers. Background Reading - Selected Internet Resources in chemistry –Major Publishers in Chemical science, Author, Citation, Computer Searching, Reviews, Keywords

**UNIT-IV : Chemical Safety and Ethical Handling of Chemicals: (12 Hrs)**

Safe working procedure and protective environment, protective apparel, emergency procedure and first aid, laboratory ventilation. Safe storage and use of hazardous chemicals, procedure for working with substances that pose hazards, flammable or explosive hazards, procedures for working with gases at pressures above or below atmospheric – safe storage and disposal of waste chemicals, recovery, recycling and reuse of laboratory chemicals, procedure for laboratory disposal of explosives, identification, verification and segregation of laboratory waste, disposal of chemicals in the sanitary sewer system, incineration and transportation of hazardous chemicals.

**UNIT-V : Data Handling (12 Hrs)**

The Investigative Approach: Making and Recording Measurements. SI Units and their use. Scientific method and design of experiments.

Analysis and Presentation of Data: Descriptive statistics. Choosing and using statistical tests. Chemo metrics. Analysis of variance (ANOVA), Correlation and regression, Curve fitting, fitting of linear equations, simple linear cases, weighted linear case, analysis of residuals, General polynomial fitting, linearizing transformations, exponential function fit, r and its abuse. Basic aspects of multiple linear regression analysis.

**Reference Books:**

- Dean, J. R., Jones, A. M., Holmes, D., Reed, R., Weyers, J. & Jones, A. (2011) Practical skills in chemistry. 2<sup>nd</sup> Ed. Prentice-Hall, Harlow.
- Hibbert, D. B. & Gooding, J. J. (2006) Data analysis for chemistry. Oxford University Press.
- Topping, J. (1984) Errors of observation and their treatment. Fourth Ed., Chapman Hall, London.
- Harris, D. C. Quantitative chemical analysis. 6<sup>th</sup> Ed., Freeman (2007) Chapters 3-5.
- Levie, R. de, how to use Excel in analytical chemistry and in general scientific data analysis. Cambridge Univ. Press (2001) 487 pages.
- Chemical safety matters – IUPAC – IPCS, Cambridge University Press, 1992.
- OSU safety manual 1.01.

**TUTORIAL / FIELD WORK / LIBRARY WORK / MODEL RESEARCH**

Students shall spend 30 Hrs for this activity under the supervision and guidance of faculty and submit a report.

**Scheme of Valuation: (Max marks: 25)**

|                              |       |          |
|------------------------------|-------|----------|
| 1. Internal Marks            | ----- | 5 marks  |
| 2. Record of activities      | ----- | 5 marks  |
| 3. Viva                      | ----- | 5 marks  |
| 4. Report submitted as above | ----- | 10 marks |

## DSC-2E: UCHM 350: INORGANIC CHEMISTRY– PRACTICAL - II

(60 Lectures)

0-1-4-2

### A. GRAVIMETRIC ANALYSIS

1. Determination of water of hydration.
2. Determination of Lead as Lead chromate (sintered glass crucible).
3. Determination of Copper as cuprous thiocyanate (sintered glass crucible).
4. Determination of Zinc (or Magnesium) as oxinate (sintered glass crucible).
5. Determination of Nickel as Ni-DMG complex (sintered glass crucible).
6. Determination of Calcium as oxalate (sintered glass crucible).
7. Determination of Iron as ferric oxide.
8. Determination of Barium as Barium sulphate (silica crucible).
9. Determination of Barium as Barium chromate (sintered glass crucible).
10. Determination of Fluoride as PbClF.

### B. PREPARATION OF INORGANIC COMPLEXES:

1. Preparation of Ni-DMG complex.
2. Preparation of Copper tetrammine complex.
3. Preparation of Lead-thiourea complex.
4. Preparation of Potassium trioxalato chromate complex.
5. Preparation of Sodium trioxalato ferrate (III)

### Scheme of Valuation: (Max marks: 50)

|   |       |                      |
|---|-------|----------------------|
| 4. Internal Marks                           | ----- | 10 marks             |
| 5. Record (containing both A & B)           | ----- | 5 marks              |
| 6. Viva                                     | ----- | 5 marks              |
| 7. Inorganic Preparation                    | ----- | 10 marks             |
| 8. Gravimetry Experiment (based on error %) | ----- | 20 marks (see below) |
| Up to 2% error                              | ----- | 20 marks             |
| 2% to 3%                                    | ----- | 16 marks             |
| 3% to 4%                                    | ----- | 12 marks             |
| 4% to 5%                                    | ----- | 8 marks              |
| More than 5% error or expt. is incomplete   | ----- | 4 marks              |

For calculation mistake: 1 marks to be deducted; for no calculation: 2 marks to be deducted.

### III – Year – Semester - V

## SEC-3: UCHM 358: GREEN METHODS IN CHEMISTRY (30 Lectures)

**Introduction:** Definitions of Green Chemistry. Brief introduction of twelve principles of Green Chemistry with examples, special emphasis on atom economy, reducing toxicity.

**Waste Production, problems and prevention:** Sources of waste, some problems caused by waste, Cost of waste, Waste minimization techniques, On-site waste treatment, Design for degradation and polymer recycling.

**Designing Green Processes:** Conventional reactors, Inherently safer design, Process intensification, In-Process monitoring.

**Industrial case studies in Green methods:** A brighter shade of green, Greening of Acetic acid manufacture, Vitamin C, Leather manufacture- tanning and fat liquoring. Dyeing to be green, Polythene-radical process and Ziegler-Natta catalysis, Eco-friendly Pesticides-Insecticides.

**Green synthesis** of poly lactic acid from Corn and Surfactants for carbon dioxide – Replacing smog producing and ozone depleting solvents with CO<sub>2</sub> for precision cleaning and dry cleaning of garments.

#### **Reference Books:**

1. Anastas, P.T. & Warner, J.K. Green Chemistry- Theory and Practical, Oxford University Press (1998).
2. Matlack, A.S. Introduction to Green Chemistry, Marcel Dekker (2001).
3. Cann, M.C. & Connely, M.E. Real-World cases in Green Chemistry, American Chemical Society, Washington (2000).
4. Ryan, M.A. & Tinnesand, M. Introduction to Green Chemistry, American Chemical Society, Washington (2002).
5. Lancaster, M. Green Chemistry: An introductory text, Green chemistry Network, University of York, The Royal Society of Chemistry (2002).

## **PRACTICALS (FOR INTERNAL ASSESSMENT ONLY):**

- 1 . Green method of  $S_N2$  reaction of 2-naphthol with Iodobutane.
2. Preparation of E and Z isomer of 1-(4-bromophenyl) -2-phenyl ethene by Wittig reaction. (Greener method)
3. Solvent less synthesis of Chalcones by Aldol condensation using Green method.
4. Preparation of 3-hydroxy-2,6-dimethyl-5-heptene from 1-chloro-3-methyl-2-butene (Grignard reaction) by Green method.
5. An efficient, green synthesis of a compostable and widely applicable plastic (poly lactic acid) made from corn.
6. Development of Fully Recyclable Carpet: Cradle to Cradle Carpeting

## **SCHEME OF EXAMINATION:**

|                               |       |  |
|-------------------------------|-------|--|
| External Theory Examination   | ----- | <b>40 marks</b> (to be conducted by University with time duration of 2 Hrs.)   |
| Internal Practical Assessment | ----- | <b>10 marks</b> (to be provided by the teacher as CIA, based on the performance of the student during practical classes) |

### III – Year – Semester - V

#### SEC-3: UCHM 359: PHARMACEUTICAL CHEMISTRY

(30 Lectures)

1-1-0-2

- To effectively impart knowledge about various diseases and their treatment.
- To know about the different types of drugs with examples.
- To learn about the importance of Indian medicinal plants.
- To learn about HIV and its treatment & prevention.

#### UNIT I - INTRODUCTION

Types of diseases - common diseases, infective diseases, insect-borne, air-borne and water-borne diseases – hereditary diseases –

Definition of the following terms: drug, pharmacophore, pharmacology, pharmacopoeia, bacteria, virus, chemotherapy and vaccine.

Drug discovery, design and development; Basic Retrosynthetic approach - absorption of drugs – factors affecting absorption – therapeutic index (Basic concepts only)

#### UNIT II- DRUGS – Classification and Action

Importance and Classification of drugs with examples – Definition and action of Antipyretics, anti-inflammatory, analgesics (Aspirin, paracetamol, Ibuprofen), antibiotics (Penicillin, Streptomycin, chloramphenicol, ampicillin), Antivirals (Acyclovir), antimetabolites, antibacterial and antifungal agents (Sulphonamides), Central Nervous System agents (Phenobarbital, Diazepam), Cardiovascular (Glycerol trinitrate)

(Structure, preparation and mode of action of the above drugs not required)

Drug receptors and biological responses – factors affecting metabolism of drugs. (Basic concepts only)

Indian medicinal plants and uses-Tulasi, Neem, Kizhanelli, Semparuthi, Adadodai and Thoothuvalai.

#### UNIT III - HEALTH PROMOTING DRUGS & HIV

Vitamins A,B, C, D, E and K - micronutrients – Na, K, Ca, Cu, Zn and I, Medicinally important inorganic compounds of Al, P, As, Hg and Fe, Examples and applications, Agents for kidney function (Aminohippuric acid). Agents for liver function (Sulfo bromophthalein), antioxidants, antacids, treatment of ulcer. (Structure not required)

HIV – symptoms, prevention, treatment – AIDS related drugs (AZT- Zidovudine)

### **RECOMMENDED TEXT BOOKS:**

1. S.Lakshmi Pharmaceutical Chemistry, S.Chand & Sons, New Delhi, 2004
2. V.K. Ahluwalia and Madhu Chopra, —Medicinal Chemistry, Ane Books, New Delhi, 2008
3. P.Parimoo, — A Text Book of Medicinal Chemistry, CBS publishers, New Delhi, 2006

### **RECOMMENDED REFERENCE BOOKS**

1. Ashutosh Kar, —Medicinal Chemistry, Wiley Eastern Ltd., New Delhi, 1993,
2. David William and Thomas Lemke, Foyes Principles of Medicinal Chemistry, BI Publishers.
3. Romas Nogrady, Medicinal Chemistry, Oxford Univ. Press
4. G.L. Patrick: Introduction to Medicinal Chemistry, Oxford University Press, UK.
5. Hakishan, V.K. Kapoor: Medicinal and Pharmaceutical Chemistry, VallabhPrakashan, Pitampura, New Delhi.
6. William O. Foye, Thomas L., Lemke, David A. William: Principles of Medicinal Chemistry, B.I. Waverly Pvt. Ltd. New Delhi.

### **PRACTICALS (FOR INTERNAL ASSESSMENT ONLY):**

1. Preparation of Aspirin and its analysis.
2. Preparation of magnesium bisilicate (Antacid).
3. Report on HIV – symptoms, prevention & treatment.
4. Report on Indian medicinal plants and their uses.

### **SCHEME OF EXAMINATION:**

|                               |       |  |
|-------------------------------|-------|--|
| External Theory Examination   | ----- | <b>40 marks</b> (to be conducted by University with time duration of 2 Hrs.)   |
| Internal Practical Assessment | ----- | <b>10 marks</b> (to be provided by the teacher as CIA, based on the performance of the student during the practical classes) |



**III Year – Semester - V**  
**CHEMISTRY- GENERIC ELECTIVE**  
**GENERIC ELECTIVE -1**

(For Other Department Students –ANY ONE OF THE THREE)

**1. Fundamentals of Chemistry & Its Application in Everyday Life**

(50 Lectures)

***Module 1: Atomic structure*** (10 hrs)

Atom model of Dalton, Thomson, Rutherford and Bohr. Nature of electron, proton and neutron – atomic number – mass number- isotopes -state the relative charges and approximate relative masses of a proton, neutron and an electron - describe, with the aid of diagrams, the structure of simple atoms as containing protons and neutrons (nucleons) in the nucleus and electrons arranged in shells (energy levels) (no knowledge of s, p, d and f orbitals);

***Module 2: Periodic table*** (10 hrs)

The Periodic Table - Periodic trends, Group properties - describe the relationship between group number and the ionic charge of an element- similarities among the elements in the same group - metallic to non-metallic character from left to right across a period of the Period Table- Properties of elements in Group I and XVII using the Periodic Table

***Module 3: Structure and properties of materials*** (10 hrs)

Elements, compounds and mixtures – elementary idea of ionic bond and covalent bond- compare the structure of simple molecular substances, e.g. methane, water, carbon dioxide, iodine, with those of giant molecular substances, e.g. poly(ethene); sand (silicon dioxide); diamond and graphite in order to deduce their properties - compare the bonding and structures of diamond and graphite , electrical conductivity.

***Module 4: Chemicals in everyday life- I*** (10 hrs)  
(No structural formula and preparation needed)

**Household materials:** Major chemical ingredients, applications, mode of action and possible hazards/toxicity of: Match Box, Household bleach, Soap, detergent, cooking gas, tooth paste, shampoo, hair dye, nail polish, perfumes, talcum powder, and moth balls – Plastics in daily use, polythene, PVC, Bakelite, polyesters and their applications.

***Module 5: Chemicals in everyday life- II*** (10 hrs)  
(No structural formula and preparation needed)

**Chemicals in food production** - Artificial sweeteners, food preservatives.

Important chemical ingredients/ taste makers used in packed food and soft drinks - its health hazards.

Adulterants in milk, ghee, oil, coffee powder, tea, asafoetida, chilli powder, pulses and turmeric powder – identification techniques (principle and outline only).

## References

1. M. C. Day and J. Selbin, "Theoretical Inorganic Chemistry".
2. F. A. Cotton, G. Wilkinson and P. L. Gaus, "Basic Inorganic Chemistry"
3. J. D. Lee, "Concise Inorganic Chemistry"
4. N.C. Datta "The Story of Chemistry"
5. Carl H. Snyder "The Extra Ordinary Chemistry Of Ordinary Things"
6. John Emsley "The Consumer's Good Chemical Guide"
7. T.P. Coultate, Food – The Chemistry of its components. Royal Society of Chemistry London, (paper back)
8. B.K. Sharma, *Polymer Chemistry*, Goel Publishing House, Meerut
9. Meyer, Food Chemistry, New Age, 2004
10. Chemistry at Home: Exploring the Ingredients in Everyday Products 1st Edition by [John Emsley](#)
11. Brannen and et al., Food Additives, Marcel Dekker, New York, 1990
12. Food Technology processing and laboratory control – Aylrand, Allied Scientific Publisher, 1999.
13. [Alfred J Shilton](#), Household Chemistry: For the Non-Chemical. (Paperback), BiblioLife
14. Food processing and preservation – Subbulakshmi, G. Shobha, A. Udipi, New Age International (P) Ltd., 2006.

## **2. Essentials of Chemistry**

**(50 Hours)**

### ***Module 1: Atomic structure and Periodic Classification of Elements*** **(10 hrs)**

Structure of atom- Fundamental particles, atomic mass, atomic number, isotopes. Bohr theory of atom. Orbitals- Quantum numbers, aufbau principle, Hund's rule; Pauli's exclusion principle. Electronic configuration of atoms- half and completely filled orbitals. Modern periodic table: Periods, Groups, Periodicity- valency, atomic radius, electronegativity, Ionisation potential, Electron affinity.

### ***Module 2 : Nuclear Chemistry*** **(10 hrs)**

Natural radioactivity, Nature and types of radiations, Properties. Group displacement law. Radio active decay series. Decay rate. Half life period, Average life period, Unit of radioactivity. Radiation dose, artificial radioactivity, nuclear structure. Nuclear fission and Nuclear fusion. Rock dating- Radio carbon dating. (*elementary idea only*)

### ***Module 3 : Polymer Chemistry*** **(10 hrs)**

Classification of polymer: Origin, structure, synthesis, Molecular forces. Commercially important polymers: Application of polyethylene, polystyrene, polyhaloolefines, Nylon-6, Nylon-66, Melamine, Terylene, Bakelite, Natural and synthetic rubber, vulcanization, inorganic polymer: (*Examples Only*).

### ***Module 4 : Chemistry in Biological Process*** **(10 hrs)**

Vitamins: Vitamin-A, Vitamin-B2, Vitamin-C, Vitamin-D, Vitamin-E and Vitamin-K- Name, Source, Function and deficiency diseases. Enzymes- Classifications, characteristics, role, examples. Hormones- Sex hormones- Androgens, oestrogens, progesterone, Example, function. Cortical hormones- A few examples with function. Nucleic acid- RNA, DNA: Introduction- role in life process (*No structure or chemical reactions needed*)

### ***Module 5 : Chemistry in action*** **(10 hrs)**

Dyes: classification based on constitution, application, examples, uses. Drugs: Antipyretic, analgesic, antiseptic, disinfectants, tranquilisers, antibiotics structure, name and uses only. Soaps and detergents: Hard and soft soaps, anionic, cationic and non-ionic detergents, cleansing action of soaps, Explosives: TNT, TNG, RDX, Gun cotton: name, structure and action. (*No structure or chemical reactions needed*)

## References

1. M. C. Day and J. Selbin, "Theoretical Inorganic Chemistry".
2. H. S. Arniker, "Essentials of Nuclear Chemistry".
3. B.K. Sharma "Environmental Pollution".
4. Solomons- John- Wiley, "Fundamentals of Organic Chemistry".
5. F.A. Carey, Mc. Graw Hill, "Organic Chemistry" Inc. 226
6. I.L Finar, "Organic Chemistry", Vol. 1 Longman
7. Tewari, Mehrotra- Vikas & Vishnoi, "A Text book for Organic Chemistry".
8. M.K. JainJain, "Principles of Organic Chemistry".

### **3. Chemistry in Everyday Life**

**(50 Hours)**

**(For Other Department Students)**

***Module I:***

***(10hrs)***

Functional food additives, adulteration, food laws. Food colours-permitted and nonpermitted – Toxicology. Flavours – natural and synthetic – Toxicology - other functional additives. Soft drinks – formulation. Health drinks.

***Module II:***

***(10hrs)***

Soaps – Introduction, detergent action of soap. Toilet soap, bathing bars, washing soaps, liquid soap manufacture – Batch process, cold process, hot process – semi boiled process, boiled process. Additives, fillers and flavours. Significances of acidity and alkalinity.

***Module III:***

***(10 hrs)***

Detergents – Introduction, Detergent action, types of detergents – cationic, anionic, amphiphilic detergents. Common detergent chemicals. Additives, excipients colours and flavours. Enzymes used in commercial detergents. Environmental Hazards.

***Module IV:***

***(10 hrs)***

Cosmetics – Introduction, classification – bathing oils. Face creams, toilet powder, skin products, dental cosmetics, hair dyes, shaving cream, shampoo. General formation for each types. Toxicology of cosmetics.

***Module V:***

***(10 hrs)***

Plastics in daily use. Polymerization process (brief). Thermosetting and thermoplastic polymers. Use of PET, HDPE, PVC, LDPE, PP, PS, ABS, and others. Recycling of plastics. Biodegradable plastics. Environmental Hazards of plastics. Paper news print, writing paper, paper boards, cardboards. Organic materials, wood, cotton, Jute, coir – International Universal recycling codes and symbols for identification.

### *References*

1. T.P. Coultate, Food – The Chemistry of its components. Royal Society of Chemistry London, (paper back)
2. Shashi Chowls, Engineering Chemistry, Darpat Rai Publication.
3. B.K. Sharma, Industrial Chemistry.
4. CNR Rao, Understanding Chemistry, Universities Press.

### III Year – Semester - VI

#### DSC – 1 F: UCHM 361: ORGANIC CHEMISTRY-II

(60 Lectures)

4-1-0-4

#### Objective:

- To study the Molecular Rearrangements
- To study the Natural Products
- To study the Carbohydrates
- To study Aminoacids, Peptides, Proteins and Nucleic acids
- To study the Application of Spectroscopy to Simple Organic Molecules

#### UNIT-I: Molecular Rearrangements:

(12 Hrs)

Classification – Types of skeletal rearrangements - anionotropic and cationotropic, inter molecular and intra molecular rearrangements - Mechanisms, evidences, migratory aptitude, inter or intra molecular of the following rearrangements: Pinacol-Pinacolone rearrangement, Hofmann rearrangement, Beckmann rearrangement, Benzil-Benzilic acid rearrangement, Baeyer-Villiger, Fries rearrangement, Claisen rearrangement, Benzidine rearrangement, Curtius rearrangement, Wagner-Meerwein rearrangement, and Wolff rearrangement.

#### UNIT –II: Natural Products:

(12 Hrs)

**Terpenoids:** Classification, nomenclature, occurrence and isolation. Isoprene rule. General method of structure determination and confirmation by synthesis, taking  $\alpha$ -terpeneol as example.

**Alkaloids:** Definition, classification, occurrence and isolation. General method of structure determination and confirmation by synthesis, taking quinine as example.

An introduction to steroids, poly-phenolics, marine natural products and their biological significance.

#### Unit – III Carbohydrates

(12 Hrs)

**Carbohydrates:** Definition, classification, configuration of aldoses & ketoses, reactions of monosaccharides (glucose, fructose), inter-conversion of glucose to fructose and vice versa, chain lengthening and chain shortening of aldoses, objections to open chain structure of glucose and fructose, mutarotation, cyclic structure of monosaccharides (glucose, fructose). Determination of ring size in glucose and fructose. Introduction to disaccharide (sucrose and maltose with structure determination) and polysaccharides (starch and cellulose without involving structure determination).

## Unit – IV: Aminoacids, Peptides, Proteins and Nucleic Acids

(12 Hrs)

**Aminoacids:** Classification, structure and stereochemistry of amino acids, isoelectric point of amino acids. Preparation and properties of alpha-amino acids – tests for amino acids.

**Peptides:** Structure and nomenclature, synthesis of polypeptides (general methods). Solid-phase peptide synthesis. Structure determination of polypeptides - end group analysis.

**Proteins:** - Classification of protein, structure of protein (determination of structure are not required). Protein denaturation, renaturation.

**Nucleic acids:** Introduction, constituents of nucleic acid, RNA and DNA, types of RNA, structure of DNA.

## UNIT - V Organic Spectroscopy

(12 hrs)

**a. UV-Visible Spectroscopy:** Basic Principles, application of UV-Visible Spectroscopy to structural elucidation of simple organic molecules, Woodward- Fieser rules, presentation and analysis of UV spectra, types of electronic transitions, effect of conjugation, concept of chromophore and auxochrome, bathochromic, hypsochromic, hyper chromic and hypochromic shifts.

**b. Infra Red Spectroscopy:** Molecular vibrations, Hook's law, selection rules, intensity and position of IR bands, measurement of IR spectrum, finger print region, characteristic absorptions of various functional groups and interpretation of IR spectra of simple organic molecules.

**c. Proton Magnetic Resonance ( $^1\text{H}$  NMR) Spectroscopy:** Magnetic and non-magnetic nuclei, nuclear shielding and de-shielding, chemical shift, spin-spin splitting and coupling constants, intensity of signals, interpretation of PMR spectra of ethyl bromide, ethanol and acetaldehyde.

### References:

- Morrison, R. T. & Boyd, R. N. Organic Chemistry, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- Finar, I. L. Organic Chemistry (Volume 1), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- Finar, I. L. Organic Chemistry (Volume 2), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- Peter Sykes: A Guide Book to Mechanism in Organic Chemistry, Orient Longman.
- ArunBahl and B. S. Bahl: Advanced Organic Chemistry, S. Chand & Company Ltd.,
- Dudley H Williams & Ian Fleming, Spectroscopic Methods in Organic Chemistry, Tata McGraw-Hill Publishing Company Ltd., (New Delhi), Fourth Edition.
- Y.R.Sharma, Elementary Organic Spectroscopy, S. Chand & Company Ltd.,



### III Year – Semester - VI

#### DSE: UCHM 362: ANALYTICAL CHEMISTRY

(60 Lectures)

4-1-0-4

#### Objective:

- To learn Flame Spectroscopic Techniques
- To learn UV-Vis. Spectroscopy
- To learn Infrared Spectroscopy
- To learn Mass Spectroscopy
- To learn NMR Spectroscopy

#### UNIT-I

(12 Hrs)

#### FLAME SPECTROMETRY

**(A) Atomic absorption spectroscopy** - Principle – elementary theory - instrumentation – Radiation sources (line sources) – Hollow cathode lamps and discharge lamps, interferences – Analytical techniques for AAS – Calibration curves.- Applications – Determination of Calcium and Magnesium in tap water – Advantages and disadvantages of AAS.

**(B) Flame Emission Spectroscopy (Flame photometry)** - Principle – Instrumentation – interferences – analytical techniques for Flame Photometry – calibration curves. Determination of Li, Na, K and Ca in water - Applications and advantages of FES - Differences between AAS and FES.

#### Unit: II

(12 Hrs)

**UV-Visible Spectroscopy:** Electromagnetic radiation, interaction of radiation with matter, quantization of different forms of energies in molecules - Definition of spectrum, Origin of spectra, fundamental laws of spectroscopy and selection rules. UV - Visible Spectroscopy - Absorption laws - validity of Beer-Lambert's law - Calculations involving Beer Lambert's law - Basic principles of instrumentation (choice of source, monochromator and detector) for single and double beam instruments - photo colorimeter and spectrophotometer- block diagrams with description of components - theory - types of electronic transitions - chromophore and auxochromes - Absorption bands and intensity - factors governing absorption maximum and intensity - Basic principles of quantitative analysis: estimation of metal ions from aqueous solution.

#### Unit: III

(12 Hrs)

**Infrared Spectroscopy:** Infrared radiation and modes of vibration of diatomic, triatomic linear (CO<sub>2</sub>) and nonlinear triatomic molecules (H<sub>2</sub>O) - stretching and bending vibrations - selection rules - functional group and fingerprint region. IR spectra of alkanes, alkenes and simple alcohols (inter and intramolecular hydrogen bonding), aldehydes, ketones, carboxylic acids and their derivatives (effect of substitution on >C=O stretching absorptions).

Basic principles of instrumentation (choice of source, monochromator & detector) for single and double beam instrument; sampling techniques. Applications of IR Spectroscopy – interpretation of the spectra of alcohols, aldehydes, ketones and esters – aliphatic and aromatic. Hydrogen bonding. Advantages of Fourier Transform (FTIR).

#### **Unit: IV**

**(12 Hrs)**

**Mass spectroscopy** - Basic principles - instrumentation - molecular ion peak, base peak, metastable peak, isotopic peak their uses. Fragmentation – Nitrogen rule - determination of molecular formulae – mass spectrum of simple organic compounds – identification – alcohols, aldehydes, aromatic hydrocarbons.

Interpretation of mass spectra of simple organic compounds such as Acetone, Anisole, Benzaldehyde, Ethyl acetate, Ethylamine, Ethyl Bromide, Toluene and Isopropyl phenyl ketone. Mc-Lefferty Rearrangement.

#### **Unit: V**

**(12 Hrs)**

**NMR Spectroscopy** - principle of nuclear magnetic resonance – basic instrumentation - number of signals - chemical shift - Factors affecting chemical shift - shielding and deshielding - Spin spin coupling and coupling constants. TMS as NMR standard.

Interpretation of NMR spectra of simple organic compounds such as Ethanol, Acetaldehyde, Acetone, Anisole, Benzaldehyde, Ethyl acetate, Ethylamine, Ethyl Bromide, Toluene and Isopropyl phenyl ketone.

#### **References:**

1. Skoog, D.A. Holler F.J. & Nieman, T.A. Principles of Instrumental Analysis, Cengage Learning India Ed.
2. Willard, H.H., Merritt, L.L., Dean, J. & Settle, F.A. Instrumental Methods of Analysis, 7<sup>th</sup> Ed. Wadsworth Publishing Company Ltd., Belmont, California, USA, 1988.
3. C.N. Banwell: Fundamentals of Molecular Spectroscopy.
4. Elements of Analytical Chemistry - R. Gopalan, P.S. Subramanian, K. Rengarajan - S. Chand and sons (1997).
5. Fundamentals of Analytical Chemistry - D.A. Skoog and D.M. West - Holt Reinhard and Winston Publication - IV Edition (1982).
6. Principles of Instrumental Methods of Analysis - D.A Skoog and Saunders - College publications - III edition (1985).
7. Analytical Chemistry - S.M. Khopkar - New Age International.
8. Instrumental Methods of Chemical Analysis - Chatwal - Anand -Himalaya Publishing House - (2000).
9. Analytical Chemistry S.Usharani, Macmillan.
10. Instrumental Methods of Analysis - Willard Merit Dean and Settle – Saunders College Publication.
11. Physico Chemical Techniques of Analysis - P.B. Janarthanam-Vol- I & II - Asian Publishing.
12. Instrumental Methods of Chemical Analysis – B.K. Sharma - Goel Publications.

## DSE: UCHM - 362: ANALYTICAL CHEMISTRY: PRACTICAL

1. Determination of a Mixture of Cobalt and Nickel (UV/Vis spec.)
2. Study the 200-500 nm absorbance spectra of  $\text{KMnO}_4$  and  $\text{K}_2\text{Cr}_2\text{O}_7$  (in 0.1 M  $\text{H}_2\text{SO}_4$ ) and determine the  $\lambda_{\text{max}}$  values. Calculate the energies of the two transitions in different units (J molecule<sup>-1</sup>, kJ mol<sup>-1</sup>, cm<sup>-1</sup>, eV).
3. Study of Electronic Transitions in Organic Molecules (i.e., acetone in water)
4. Study the pH-dependence of the UV-Vis spectrum (200-500 nm) of  $\text{K}_2\text{Cr}_2\text{O}_7$ .
5. Record the 200-350 nm UV spectra of the given compounds (acetone, acetaldehyde, 2-propanol, acetic acid) in water. Comment on the effect of structure on the UV spectra of organic compounds.
6. Verify Lambert-Beer's law and determine the concentration of  $\text{CuSO}_4/\text{KMnO}_4/\text{K}_2\text{Cr}_2\text{O}_7$  in a solution of unknown concentration
7. Determine the concentrations of  $\text{KMnO}_4$  and  $\text{K}_2\text{Cr}_2\text{O}_7$  in a mixture
8. Preparation of acetylacetonato complexes of  $\text{Cu}^{2+}/\text{Fe}^{3+}$ . Find the  $\lambda_{\text{max}}$  of the complex
9. IR Absorption Spectra (Study of Aldehydes and Ketones)
10. Determination of Calcium, Iron, and Copper in Food by Atomic Absorption
11. Determine the pH of the given aerated drinks fruit juices, shampoos and soaps.
12. Determination of Na, Ca, Li in cola drinks and fruit juices using flame photometric techniques.
13. Estimation of calcium, magnesium, phosphate, nitrate
14. Determination of pKa values of indicator using spectrophotometry.
15. Structural characterization of compounds by infrared spectroscopy.
16. Identification of simple organic compounds by IR spectroscopy and NMR spectroscopy (Spectra to be provided).

### Reference Books

1. Khosla, B. D.; Garg, V. C. & Gulati, A., *Senior Practical Physical Chemistry*, R. Chand & Co.: New Delhi (2011).
2. Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. *Experiments in Physical Chemistry 8th Ed.*; McGraw-Hill: New York (2003).
3. Halpern, A. M. & McBane, G. C. *Experimental Physical Chemistry 3rd Ed.*; W.H. Freeman & Co.: New York (2003).
4. Vogel's *Qualitative Inorganic Analysis*, Revised by G. Svehla.
5. Marr & Rockett *Inorganic Preparations*

### Scheme of Valuation: (Max marks: 25)

|  |       |          |
|--|-------|----------|
| 9. Internal Marks                          | ----- | 5 marks  |
| 10. Record                                 | ----- | 5 marks  |
| 11. Viva                                   | ----- | 5 marks  |
| 12. Any one experiment from the above list | ----- | 10 marks |

## DSE: UCHM - 363: POLYMER CHEMISTRY

(60 Lectures)

4-1-0-4

### Objective:

- To learn the classification of polymers
- To learn the Polymerization reactions
- To learn the properties of polymers
- To learn polymerization techniques and polymer degradation
- To learn the chemistry of commercial polymers

### UNIT-I INTRODUCTION AND CLASSIFICATION OF POLYMERS:

Definition of monomer, oligomer and polymer; Different schemes of classification of polymers – Natural, synthetic - linear, cross linked and network - distinction between plastics, elastomers and fibres; Rate of polymerization; degree of polymerization. Homo and hetero polymers, copolymers, Natural polymers- cellulose, silk, gums and resin . Types of plastics- thermoplastics and thermosetting plastics, functionality concept - Concept of cross linked polymers.

### UNIT-II POLYMERIZATION REACTIONS:

Types of polymerization reactions - addition, condensation, ionic, co-ordination.

Addition polymerisation – mechanism, initiation, propagation and termination processes, initiators, inhibitors.

Mechanism and kinetics of step growth, radical chain growth, ionic chain (both cationic and anionic) and condensation polymerizations, Mechanism and kinetics of copolymerization and emulsion polymerization techniques.

:

### UNIT-III PROPERTIES OF POLYMERS:

Physical, thermal, flow & mechanical properties of polymers, glass transition temp. ( $T_g$ ) - definition, factors affecting  $T_g$ , Relationship between  $T_g$  and molecular weight. - crystalline melting point and degree of crystallinity – Structure-Property relationships.

Concept of average molecular weight of polymers; molecular weight distribution; Absolute and relative methods of molecular mass determination - number average, weight average, and viscosity average molecular weight; molecular weight determination by osmometry method, light scattering method, sedimentation method, ultra centrifugation, and viscosity method (principles only - No experimental details expected).

#### **UNIT-IV POLYMERIZATION TECHNIQUES AND POLYMER DEGRADATION:**

(a) Polymerization techniques: Bulk, solution, suspension & emulsion polymerization - melt polycondensation. Polymer processing - compression moulding, casting, extrusion, fibre spinning, injection moulding, thermoforming, vulcanization of elastomers, Polymer processing.

(b) Polymer degradation: thermal, mechanical, oxidative and chemical methods and biodegradation.

#### **UNIT-V CHEMISTRY OF COMMERCIAL POLYMERS:**

General methods of preparation, properties and uses of the following: polyethylene, polystyrene, polyesters, polyamides, polycarbonates, PVC, Teflon, acrylic polymers – Phenol formaldehyde resins (Bakelite and Novolac), polyurethanes and silicone polymers - Advances in polymers - Bio-Polymers, biomaterials, polymers in medical field, High temperature and fire resistant polymers – Conducting and semiconducting polymers [polyacetylene, polyaniline, poly(p-phenylenesulphide), polypyrrole, polythiophene)].

#### **Reference Books:**

1. Billmeyer, F.W., Textbook of Polymer Science, John Wiley & Sons 1984
2. Gowariker. V.R. Viswanathan, N.V. Jayader Sreedhar, Polymer Science, Wiley Eastern Ltd., New Delhi, 2005
3. Ghosh, P., Polymer Science & Technology, Tata McGraw-Hill Education, 1991.
4. Lenz, R.W. Organic Chemistry of Synthetic High Polymers. Interscience Publishers, New York, 1967.
5. Sharma.B.K, Polymer Chemistry, Goel Publishing House, Meerut- 1989
6. Arora M.G. Vadar M.S, Polymer Chemistry, Anmol publications (p) Ltd., New Delhi 1989
7. Odian, G. Principles of Polymerization, 4<sup>th</sup> Ed. Wiley, 2004.
8. Stevens M.P., Polymer Chemistry - An introduction, 3<sup>rd</sup> Ed., Oxford University Press, 1999
9. Gowariker.V.R, Viswanathan.N.V and Sreethan.J., "Polymer Science", Wiley Eastern Ltd, 1986

## DSE: UCHM - 363: POLYMER CHEMISTRY - PRACTICAL

(60 Lectures)

0-1-4-2

### I. Polymer synthesis

1. Free radical solution polymerization of styrene (St) / Methyl Methacrylate (MMA) / Methyl Acrylate (MA) / Acrylic acid (AA) involving
  - a. Purification of monomer
  - b. Polymerization using benzoyl peroxide (BPO)/ 2,2'-azo-bis- isobutyronitrile (AIBN)
2. Preparation of nylon 66/6
3. Interfacial polymerization, preparation of polyester from isophthaloyl chloride (IPC) and phenolphthalein consisting of the following steps:
  - a. Preparation of IPC
  - b. Purification of IPC
  - c. Interfacial polymerization
4. Redox polymerization of acrylamide
5. Precipitation polymerization of acrylonitrile
6. Preparation of urea-formaldehyde resin
7. Preparation of novalac resin.

### II. Polymer characterization

8. Determination of molecular weight by viscometry:
  - (a) Polyacrylamide-aq.  $\text{NaNO}_2$  solution
  - (b) Poly vinyl propylidene (PVP) in water
9. Determination of the viscosity-average molecular weight of poly(vinyl alcohol) (PVOH)
10. Determination of molecular weight by end group analysis: Polyethylene glycol (PEG) (OH group).
11. Testing of mechanical properties of polymers.
12. Determination of hydroxyl number of a polymer using colorimetric method.

**Reference Books:**

- M.P. Stevens, Polymer Chemistry: An Introduction, 3<sup>rd</sup> Ed., Oxford University Press, 1999.
- H.R. Allcock, F.W. Lampe & J.E. Mark, Contemporary Polymer Chemistry, 3rd ed. Prentice-Hall (2003)
- F.W. Billmeyer, Textbook of Polymer Science, 3<sup>rd</sup> ed. Wiley-Interscience (1984)
- J.R. Fried, Polymer Science and Technology, 2<sup>nd</sup> ed. Prentice-Hall (2003)
- P. Munk & T.M. Aminabhavi, Introduction to Macromolecular Science, 2<sup>nd</sup> ed. John Wiley & Sons (2002)
- L. H. Sperling, Introduction to Physical Polymer Science, 4<sup>th</sup> ed. John Wiley & Sons (2005)
- Seymour/ Carraher's Polymer Chemistry, 9<sup>th</sup> ed. by Charles E. Carraher, Jr. (2013).

**Scheme of Valuation: (Max marks: 25)**

|   |       |          |
|---|-------|----------|
| 1. Internal Marks                         | ----- | 5 marks  |
| 2. Record                                 | ----- | 5 marks  |
| 3. Viva                                   | ----- | 5 marks  |
| 4. Any one experiment from the above list | ----- | 10 marks |

## **DSE: UCHM - 364: MOLECULAR MODELLING & DRUG DESIGN**

**(60 Lectures)**

**4-1-0-4**

### **Objective:**

- To learn the basics of molecular modelling
- To learn the force fields
- To learn the energy minimization and computer simulation
- To learn molecular dynamics & Monte Carlo simulation
- To learn the structure prediction and drug design

### **UNIT-I : Introduction to Molecular Modelling:**

**(12 Hrs)**

Introduction. Useful Concepts in Molecular Modelling: Coordinate Systems. Potential Energy Surfaces. Molecular Graphics. Surfaces. Computer Hardware and Software. The Molecular Modelling Literature.

### **UNIT-II : Force Fields:**

**(12 Hrs)**

Fields. Bond Stretching. Angle Bending. Introduction to nonbonded interactions. Electrostatic interactions. van der Waals Interactions. Hydrogen bonding in Molecular Mechanics. Force Field Models for the Simulation of Liquid Water.

### **UNIT-III : Energy Minimization and Computer Simulation:**

**(12 Hrs)**

Minimization and related methods for exploring the energy surface. Non-derivative method, First and second order minimization methods. Computer simulation methods. Simple thermodynamic properties and Phase Space. Boundaries. Analyzing the results of a simulation and estimating Errors.

### **UNIT-IV : Molecular Dynamics & Monte Carlo Simulation:**

**(12 Hrs)**

Molecular Dynamics Simulation Methods. Molecular Dynamics using simple models. Molecular Dynamics with continuous potentials. Molecular Dynamics at constant temperature and pressure. Metropolis method. Monte Carlo simulation of molecules. Models used in Monte Carlo simulations of polymers.

### **UNIT-V : Structure Prediction and Drug Design:**

**(12 Hrs)**

Structure prediction – Introduction to comparative Modelling. Sequence alignment. Constructing and evaluating a comparative model. Predicting protein structures by 'Threading', Molecular docking. Structure based de novo ligand design,

Drug Discovery – Chemo informatics – QSAR.



## Reference Books:

- Leach, A.R. Molecular Modelling Principles and Application, Longman, 2001.
- Haile, J.M. Molecular Dynamics Simulation Elementary Methods, John Wiley and Sons, 1997.
- Gupta, S.P. QSAR and Molecular Modelling, Springer - Anamaya Publishers, 2008.

## DSE: UCHM - 364: MOLECULAR MODELLING & DRUG DESIGN- PRACTICAL

(60 Lectures)

0-1-4-2

1. Compare the optimized C-C bond lengths in ethane, ethene, ethyne and benzene. Visualize the molecular orbitals of the ethane  $\sigma$  bonds and ethene, ethyne, benzene and pyridine  $\pi$  bonds.
2. (a) Perform a conformational analysis of butane.  
(b) Determine the enthalpy of isomerization of cis and trans 2-butene.
3. Visualize the electron density and electrostatic potential maps for LiH, HF, N<sub>2</sub>, NO and CO and comment. Relate to the dipole moments. Animate the vibrations of these molecules.
4. (a) Relate the charge on the hydrogen atom in hydrogen halides with their acid character.  
(b) Compare the basicities of the nitrogen atoms in ammonia, methylamine, dimethylamine and trimethylamine.
5. (a) Compare the shapes of the molecules: 1-butanol, 2-butanol, 2-methyl-1-propanol, and 2-methyl-2-propanol. Note the dipole moment of each molecule.  
(b) Show how the shapes affect the trend in boiling points: (118 °C, 100 °C, 108 °C, 82 °C, respectively).
6. Build and minimize organic compounds of your choice containing the following functional groups. Note the dipole moment of each compound: (a) alkyl halide (b) aldehyde (c) ketone (d) amine (e) ether (f) nitrile (g) thiol (h) carboxylic acid (i) ester (j) amide.
7. (a) Determine the heat of hydration of ethylene.  
(b) Compute the resonance energy of benzene by comparison of its enthalpy of hydrogenation with that of cyclohexene.
8. Arrange 1-hexene, 2-methyl-2-pentene, (E)-3-methyl-2-pentene, (Z)-3-methyl-2-pentene, and 2,3-dimethyl-2-butene in order of increasing stability and justify.
9. (a) Compare the optimized bond angles H<sub>2</sub>O, H<sub>2</sub>S, H<sub>2</sub>Se.  
(b) Compare the HAH bond angles for the second row dihydrides and compare with the results from qualitative MO theory.

**Note:** Software: ChemSketch, ArgusLab ([www.planaria-software.com](http://www.planaria-software.com)), TINKER 6.2 ([dasher.wustl.edu/ffe](http://dasher.wustl.edu/ffe)), WebLab Viewer, Hyperchem, or any similar software.

**Reference Books:**

- Leach, A.R. Molecular Modelling Principles and Application, Longman, 2001.
- Haile, J.M. Molecular Dynamics Simulation Elementary Methods, John Wiley and Sons, 1997.
- Gupta, S.P. QSAR and Molecular Modeling, Springer - Anamaya Publishers, 2008.

**Scheme of Valuation: (Max marks: 25)**

|   |       |          |
|---|-------|----------|
| 1. Internal Marks                         | ----- | 5 marks  |
| 2. Record                                 | ----- | 5 marks  |
| 3. Viva                                   | ----- | 5 marks  |
| 4. Any one experiment from the above list | ----- | 10 marks |

## **DSE: UCHM - 365: INDUSTRIAL CHEMICALS AND ENVIRONMENT**

**(60 Lectures)**

**4-1-0-4**

### **Objective:**

- To learn about industrial gases and inorganic chemicals
- To learn about air pollution
- To learn about water pollution
- To learn about noise pollution and radioactive pollution
- To learn about environment and energy

### **Unit – I: Industrial Gases and Inorganic Chemicals**

**(12 Hrs)**

Industrial Gases: Large scale production, hazards in storage and handling of the following gases: oxygen, nitrogen, argon, neon, helium, hydrogen, acetylene, carbon monoxide, chlorine, fluorine, sulphur dioxide and phosgene.

Inorganic Chemicals: Hazards in handling the following chemicals: hydrochloric acid, nitric acid, sulphuric acid, caustic soda, bleaching powder, sodium thiosulphate, hydrogen peroxide, potash alum, chrome alum and potassium dichromate.

### **Unit – II: Air Pollution**

**(12 Hrs)**

Air Pollution: Air pollutants: types, sources, particle size and chemical nature; Photochemical smog: its constituents and photochemistry. Pollution by SO<sub>2</sub>, CO<sub>2</sub>, CO, NO<sub>x</sub>, H<sub>2</sub>S and other foul smelling gases and control procedures – air pollution due to automobile exhausts.

Effects of air pollution on living organisms and vegetation. Greenhouse effect and Global warming, Ozone depletion by oxides of nitrogen, chlorofluorocarbons and Halogens, removal of sulphur from coal. Control of particulates.

### **Unit – III: Water Pollution:**

**(12 Hrs)**

Hydrological cycle, water resources, aquatic ecosystems, Sources and nature of water pollutants – Impacts of water pollution on hydrological and ecosystems.

Pollution of water by pesticides – Marine oil pollution – sources – effects – control; Thermal pollution – causes – effects and control; Pollution of water by soaps and detergents – classification – environmental implications – abatement procedures.

Industrial waste management, incineration of waste. Effluent treatment plants (primary, secondary and tertiary treatment). Industrial effluents from the following industries and their treatment: electroplating, textile, tannery, dairy, petroleum and petrochemicals, agro, fertilizer, etc. – Sludge disposal.

**Unit – IV: Noise Pollution and Radio active Pollution:****(12 Hrs)**

Sound and its general features – human acoustics – noise and its measurement (dB) –noise classification – effect of noise – brief discussion on control of industrial noise pollution (detailed discussion and control methods are not required)

Definitions of radioactive pollution and its units – Curie, Roentgen, Rad, Gray, Re , RBE – Sources of radiations – effects of radiations – Somatic effects – Genetic effects.

**Unit – V: Environment & Energy****(12 Hrs)**

Ecosystems. Biogeochemical cycles of carbon, nitrogen and sulphur.

Sources of energy: Coal, petrol and natural gas. Nuclear Fusion / Fission, Solar energy, Hydrogen, geothermal, Tidal and Hydel, etc.

Nuclear Pollution: Disposal of nuclear waste, nuclear disaster and its management.

Introduction to biocatalysis: Importance in “Green Chemistry” and in Chemical Industries with examples.

**Reference Books:**

- E. Stocchi: Industrial Chemistry, Vol-I, Ellis Horwood Ltd. UK.
- R.M. Felder, R.W. Rousseau: Elementary Principles of Chemical Processes, Wiley Publishers, New Delhi.
- J. A. Kent: Riegel’s Handbook of Industrial Chemistry, CBS Publishers, New Delhi.
- S. S. Dara: A Textbook of Engineering Chemistry, S. Chand & Company Ltd. New Delhi.
- K. De, Environmental Chemistry: New Age International Pvt., Ltd, New Delhi.
- S. M. Khopkar, Environmental Pollution Analysis: Wiley Eastern Ltd, New Delhi.
- S.E. Manahan, Environmental Chemistry, CRC Press (2005).
- G.T. Miller, Environmental Science 11<sup>th</sup> edition. Brooks/ Cole (2006).
- A. Mishra, Environmental Studies. Selective and Scientific Books, New Delhi (2005).

## DSE: UCHM – 365: INDUSTRIAL CHEMICALS & ENVIRONMENT -PRACTICAL

(60 Lectures)

0-1-4-2

1. Study of some of the common bio-indicators of pollution.
2. Measurement of dissolved CO<sub>2</sub>
3. Estimation of SPM in air samples.
4. Determination of acetic acid content in Vinegar by titration with NaOH.
5. Determination of alkali content in antacid tablets by titration with HCl.
6. Determination of copper content in brass by Iodoametric titration.
7. Determination of available chlorine in bleaching powder.
8. Determination of dissolved oxygen in water
9. Determination of Chemical Oxygen Demand (COD)
10. Determination of Biological Oxygen Demand (BOD)
11. Determination of hardness of water
12. Percentage of available chlorine in bleaching powder
13. Determination of Mn content in Pyrolusite
14. Measurement of chloride, sulphate and salinity of water samples by simple titration method (AgNO<sub>3</sub> and potassium chromate).
15. Estimation of total alkalinity of water samples (CO<sub>3</sub><sup>2-</sup>, HCO<sub>3</sub><sup>-</sup>) using double titration method.
16. Synthesis of Chalcone by green chemical method (condensation of benzaldehyde and acetophenone)

### Reference Books:

- E. Stocchi: Industrial Chemistry, Vol-I, Ellis Horwood Ltd. UK.
- R.M. Felder, R.W. Rousseau: Elementary Principles of Chemical Processes, Wiley Publishers, New Delhi.
- J. A. Kent: Riegel's Handbook of Industrial Chemistry, CBS Publishers, New Delhi.
- S. S. Dara: A Textbook of Engineering Chemistry, S. Chand & Company Ltd. New Delhi.
- K. De, Environmental Chemistry: New Age International Pvt. Ltd, New Delhi.
- S. M. Khopkar, Environmental Pollution Analysis: Wiley Eastern Ltd, New Delhi.

**Scheme of Valuation: (Max marks: 25)**

|   |       |          |
|---|-------|----------|
| 1. Internal Marks                       | ----- | 5 marks  |
| 2. Record                               | ----- | 5 marks  |
| 3. Viva                                 | ----- | 5 marks  |
| 4. Any one activity from the above list | ----- | 10 marks |

**DSE: UCHM – 366: DISSERTATION**

**(60 Lectures)**

**4-1-0-5**

The title/specialization of the projects and the mentor/student allotment would be decided in the department level faculty meeting. Students are required to work under their mentor on a specific novel topic.

At the end of the semester, students need to submit dissertation. The dissertation will be assessed by the committee members consist of one external member appointed by the university, head of the department and the course teacher (mentor) who offered this course. The project may be assessed based on the merit of the work, volume of the work, viva and knowledge of the student in the specific topic.

**Scheme of Valuation: (Max marks: 100)**

|                            |       |          |
|----------------------------|-------|----------|
| 1. Internal Marks          | ----- | 25 marks |
| 2. Viva                    | ----- | 25 marks |
| 3. Dissertation evaluation | ----- | 50 marks |

## DSC-2F: UCHM - 360: ORGANIC CHEMISTRY PRACTICAL-II

(60 Lectures)

0-1-4-2

### A. Organic Qualitative Analysis/

- (i) Basic idea on the preparation of reagents used in organic analysis.  
(Borshes reagent, Schiff's reagent, phenolphthalein, Neutral FeCl<sub>3</sub>, Tollens reagent, Fehlings solution)
- (ii) Study of reactions of common functional groups.
- (iii) Systematic Qualitative Analysis of organic compounds containing the following mono functional groups:  
Carbohydrate, carboxylic acid, dicarboxylic acid, phenol, aldehyde, ketone, aromatic primary amine, aromatic amide, aliphatic diamide, and nitro compound.
  - 1. Detection of nitrogen, sulphur and halogens.
  - 2. Tests to find whether saturated or unsaturated.
  - 3. Tests to find whether aromatic or aliphatic.
  - 4. Tests to find the functional group.
  - 5. Confirmation of functional group by preparation of derivatives.

### B. Organic Preparations:

- 1. Acetylation of salicylic acid.
- 2. Acetylation of aniline.
- 3. Benzoylation of aniline / phenol.
- 4. Preparation of Iodoform from ethanol / acetone.
- 5. Preparation of S-benzyl isothiuronium chloride
- 6. Preparation of m-dinitrobenzene.
- 7. Preparation of benzoic acid from benzaldehyde.

### **Reference Books:**

- 1. Vogel's Textbook of Practical Organic Chemistry, ELBS.
- 2. B.S.Furnis, A.J.Hannaford, P.W.G.Smith and T.R.Tatchell *Vogel's Text book of Practical Organic Chemistry* ELBS/Longman 1989.
- 3. S.P. Bhattani & Aruna Chhikara, *Practical organic chemistry* (qualitative analysis) Ane books (India) Pvt Ltd, 2008.
- 4. O.P. Pandey, D.N Bajpai, S. Gini, *Practical Chemistry*, for I, II & III BSc. Students. S.Chand & Company Ltd reprint 2009.

5. V.K.Ahluwalia, Sunitha Dhingra, Adarsh Gulate, *College Practical Chemistry*, Universities Press (India) Pvt Ltd 2008 (reprint)
6. V.K.Ahluwalia & Aggarwal, R. *Comprehensive Practical Organic Chemistry*, Universities Press
7. P.R.Singh, D.C.Gupta, K.S.Bajpal *Experimental Organic Chemistry* Vol.I and II, 1980.

**Scheme of Valuation: (Max marks: 50)**

|                                   |       |          |
|-----------------------------------|-------|----------|
| 1. Internal Marks                 | ----- | 10 marks |
| 2. Record (containing both A & B) | ----- | 5 marks  |
| 3. Viva                           | ----- | 5 marks  |
| 4. Organic Preparation            | ----- | 10 marks |
| 5. Organic Qualitative Analysis   | ----- | 20 marks |



### III – Year – Semester - VI

#### SEC-4: UCHM 367: FORENSIC CHEMISTRY

(30 Lectures)

1-1-0-2

#### Objective:

- To learn about transportation and types of evidence
- To learn about crime detection
- To learn about forgery and counterfeiting

#### UNIT – I: TRANSPORTATION & TYPES OF EVIDENCE (10 hrs)

Drunken driving: breath analyzer for ethanol. Incendiary and time bombs in road and railway tracks. Defusing live bombs.

Hit -and-go traffic accidents : paint analysis by AAS. Spill of toxic and corrosive chemicals (e.g., conc. acids) from tankers.

Types of evidence to prove guilty of the crime - anecdotal evidence, testimonial evidence, statistical evidence, and analogical evidence.

#### UNIT – II: CRIME DETECTION (10 hrs)

Accidental explosions during manufacture of matches and fire-works (as in Sivakasi). Human bombs, possible explosives (gelatin sticks, RDX). Metal detector devices and other security measures for VVIP. Composition of bullets and detection of powder burns.

Scene of crime: finger prints and their matching using computer records. Smell tracks and police dogs. Analysis of blood and other body fluids in rape cases. Typing of blood. DNA finger printing for tissue identification in dismembered bodies. Blood stains on clothing. Cranial analysis (head and teeth).

#### UNIT – III: FORGERY AND COUNTERFEITING (10 hrs)

Detecting forgery in bank cheques / drafts and educational records (mark lists, certificates), using UV-light. Alloy analysis using AAS to detect counterfeit coins. Checking silverline water mark in currency notes.

Jewellery : detection of gold purity in 22 carat ornaments, detecting gold plated jewels, authenticity of diamonds (natural, synthetic, glassy).

Detecting steroid consumption among athletes and race horses.

**Reference Book:**

1. Max M Houck, Forensic Chemistry, Jan.2015, Academic Press
2. Kelly M. Elkins, Introduction to Forensic Chemistry, 1<sup>st</sup> edition Oct.2018, CRC Press
3. Richard Saferstein, Criminalistics: An Introduction to Forensic Science, tenth edition
4. Vernon Geberth, Practical homicide investigation, Fifth Edition, CRC Press
5. Jay A. Siegel, Forensic Chemistry: Fundamentals and Applications, Oct. 2015, Google Books.
6. Donnell R. Christian, Jr., JaVed I. Khan, and Thomas J. Kennedy, Basic Principles of Forensic Chemistry, Nov.2011, Google Books.

**PRACTICALS (FOR INTERNAL ASSESSMENT ONLY):**

Following activities may be given to students and submit report, based on which internal practical marks can be awarded.

1. The 4 types of evidence in order to prove the person guilty of the crime. These include anecdotal evidence, testimonial evidence, statistical evidence, and analogical evidence.
2. How ink can help forensic scientists to catch criminals.
3. Do twins have identical or similar fingerprints?
4. Fingerprint Similarity Between Siblings and Non-related People
5. Build Your Own Lie-Detector / Polygraph
6. Create a DNA Fingerprint
7. Protein Identification through immunoassay.
8. TLC on various inks to determine an unknown ink sample
9. TLC on lipstick samples, then match an unknown sample to one of the knowns

**Reference:**

<https://www.juliantrubin.com/forensicprojects.html>

<https://www.juliantrubin.com/fairprojects/forensicscience/forensicscience.html>

### III – Year – Semester - VI

#### SEC-4: UCHM 368: FUEL CHEMISTRY

(30 Lectures)

1-1-0-2

#### Objective:

- To learn about energy sources and coal
- To learn about petroleum and petrochemical industry
- To learn about lubricants

#### Unit-I:

(10 hrs)

Review of energy sources (renewable and non-renewable). Classification of fuels and their calorific value.

**Coal:** Uses of coal (fuel and nonfuel) in various industries, its composition, carbonization of coal. Coal gas, producer gas and water gas—composition and uses. Fractionation of coal tar, uses of coal tar based chemicals, requisites of a good metallurgical coke, Coal gasification (Hydro gasification and Catalytic gasification), Coal liquefaction and Solvent Refining.

#### Unit-II

(10 hrs)

**Petroleum and Petrochemical Industry:** Composition of crude petroleum, Refining and different types of petroleum products and their applications.

Fractional Distillation (Principle and process), Cracking (Thermal and catalytic cracking), Reforming Petroleum and non-petroleum fuels (LPG, CNG, LNG, bio-gas, fuels derived from biomass), fuel from waste, synthetic fuels (gaseous and liquids), clean fuels. Petrochemicals: Vinyl acetate, Propylene oxide, Isoprene, Butadiene, Toluene and its derivatives - Xylene.

#### Unit-III

(10 hrs)

**Lubricants:** Classification of lubricants, lubricating oils (conducting and non-conducting) Solid and semisolid lubricants, synthetic lubricants.

Properties of lubricants (viscosity index, cloud point, pour point) and their determination.

#### Reference Books:

- Stocchi, E. Industrial Chemistry, Vol-I, Ellis Horwood Ltd. UK (1990).
- Jain, P.C. & Jain, M. Engineering Chemistry Dhanpat Rai & Sons, Delhi.
- Sharma, B.K. & Gaur, H. Industrial Chemistry, Goel Publishing House, Meerut (1996)

**III Year – Semester - VI**  
**CHEMISTRY- GENERIC ELECTIVE**  
**GENERIC ELECTIVE -2**

(For Other Department Students – ANY ONE OF THE TWO)

**1. CHEMISTRY IN AGRICULTURE**

(50 Hours)

*Module 1: Soil properties and Reactions* (10 hrs)

**Soil properties:** Definition of soil, soil composition, inorganic properties of soil, organic matters of soil - Fertilizers & Manures: Definition – differences between fertilizers and manures.

**Soil reactions:** Soil acidity, actual acidity, soil pH and its determination, buffer action capacity of soils – effects of pH on availability of N,P,K and Ca – Acid soil, alkaline soil – their formation and reclamation.

*Module 2: Nitrogen Fertilizers* (10 hrs)

Nitrogen in plant nutrition – importance of nitrogenous fertilizers – classification – ammonia – ammonium fertilizers – ammonium sulphate, ammonium nitrate, ammonium chloride.

Nitrate fertilizers – sodium nitrate, calcium nitrate, calcium ammonium nitrate (CAN), urea (outline of manufacture) and calcium cyanamide.

*Module 3: Phosphatic Fertilizers* (10 hrs)

Phosphorus in the life of plants-importance of phosphatic fertilizers. types of phosphatic fertilizers – outline of the production of calcium superphosphate, calcium metaphosphate, calcium superphosphate nitrate, triplesuperphosphate, ammoniated superphosphate, DAP, TAP, bone meal and basic slag.

*Module 4: Potassium & Complex Fertilizers* (10 hrs)

**Potassium fertilizers:** Potassium in life of plants – Deficiency symptoms – classification of potassium fertilizers – outline of the production of KCl, KNO<sub>3</sub>, K<sub>2</sub>SO<sub>4</sub> and other slags.

**Complex fertilizers:** Complete and incomplete fertilizers, manufacture of NPK fertilizers-calculation of fertilizer formula – secondary nutrients and micro nutrients – their function in plants.

***Module 5: Bio fertilizers & Plant protection chemicals***

***(10 hrs)***

Biofertilizers – Biological control of pests – integrated pest management (IPM) – Genetically modified crops – outline of the process of modifying – their advantages and disadvantages. Plant protection chemicals – definition of toxicity and LD<sub>50</sub> values.

Pesticides – Insecticides, Fungicides, Herbicides, Acaricides – definition with examples – Preparation and uses of some pesticides: DDT, BHC (Gammexane), Chlordane, Dithiocarbamates, Dalapon, Alachlor, Parathion, Malathion – general methods of application – Safety measures when using pesticides

**REFERENCE BOOKS:**

1. Soil Science by Dr. A. Shankaran
2. The nature and properties of soil by Nyle Brady
3. Chemistry of insecticides and fungicides by U.S. Sreeramulu
4. Bio fertilisers in agriculture by N.S.Subbarao.

## **2. FOOD AND MEDICINAL CHEMISTRY**

**(50 Hours)**

### ***Module-I FOOD & FOOD POISONING***

Sources of food, types, advantages and disadvantages, constituents of food, carbohydrate, protein, fats and oils, vitamins and minerals, food additives, natural toxicants.

Food Poisoning: Sources, causes and remedy – Causes and remedies for acidity, gastritis, indigestion and constipation.

### ***Module -II FOOD PRESERVATION, PROCESSING & NATURAL FOOD***

Food spoilage, courses of food spoilage, types of food spoilage, food preservation - Preservation and processing by heating- sterilization, pasteurization – Importance of Natural Food, Concept of “Food as medicine”.

### ***Module- III DRUGS***

Classification of drugs – biological & chemical (Structure not required) - Definition and two examples each (Structure not required): Anesthetics (General and local), Analgesics, Antipyretics and anti inflammatory agents – Antibiotics – Penicillin, Streptomycin, Antivirals. AIDS – symptoms, prevention & treatment – Drug receptors and biological responses – factors affecting metabolism of drugs. (Basic concepts only)

### ***Module- IV DRUGS FOR SOME CLINICAL CONDITIONS***

Diabetes – Causes, hyper and hypoglycemic drugs – Blood pressure – Systolic & Diastolic Hypertensive drugs – Cardiovascular drugs – depressants and stimulants – Lipid profile – HDL, LDL cholesterol lipid lowering drugs. (Structure not required) - Pharmacologically active constituents in plants, Indian medicinal plants – Tulsi, Neem, Keezhanelli – their importance.

**Module- V**

**HEALTH PROMOTING DRUGS**

Vitamins A,B, C, D, E and K, micronutrients – Na, K, Ca, Cu, Zn and I, Medicinally important inorganic compounds of Al, P, As, Hg and Fe, Examples and applications, Agents for kidney function (Aminohippuric acid) - Agents for liver function (Sulfo bromophthalein), antioxidants, treatment of ulcer and skin diseases (Structure not required).

**REFERENCE BOOKS:**

1. Seema Yadav, Food Chemistry, Anmol publishing (P) Ltd., New Delhi.
2. Car H. Synder, The Extraordinary Chemistry for ordinary things, John Wiley & sons inc., New York, 1992.
3. Sivasankar, Food Processing and Preservation PHI. (Eastern Economy Editions)
4. V.K. Ahluwalia and Madhu Chopra, Medicinal Chemistry, Ane Books, New Delhi, 2008
5. P. Parimoo, A Text Book of Medicinal Chemistry, CBS publishers, New Delhi, 2006
6. S.Lakshmi Pharmaceutical Chemistry, S.Chand & Sons, New Delhi, 2004
7. Ashutosh Kar, Medicinal Chemistry, Wiley Eastern Ltd., New Delhi, 1993
8. Romas Nogrady, Medicinal Chemistry, Oxford Univ. Press
9. David William and Thomas Lemke, Foyes, Principles of Medicinal Chemistry, BI Publishers