## RANI DURGAVATI UNIVERSITY, JABALPUR

## SYLLABUS FOR M.Sc. CHEMISTRY (A FOUR SEMESTERS COURSE)

## Choice Based Credit System Syllabus: Effective from July 2018 and onward

#### **COURSE STRUCTURE AND SCHEME OF EXAMINATION**

The M.Sc. Chemistry shall have 4 semesters. The number of theory papers and practical courses, along with their credit system are given in page 3. It is necessary to secure minimum 35% pass marks with Grade Point 4 separately in each theory paper and practical courses in each semester. It is also necessary to secure minimum 35% marks with Grade Point 4 in Continuous Evaluation (CE) in each semester to qualify to appear in subsequent full examination of the respective semester. The Course is governed by the **University Ordinance No. 222.** 

## Continuous Evaluation: Semesters I to IV.

- (i) In each semester, each theory course will be assessed for 100 marks, out of which 60 marks will be for end semester examination and 40 marks will be for continuous evaluation. In case of laboratory/project work based courses, appropriate distribution of marks for practical record/Attendance/ Viva-Voce/ Project report are given at the appropriate place of the syllabus. The project may be undertaken in any of the national Laboratories/Institutes/Universities/ Govt. approved Companies/Industries/ in own Department.
- (ii) During the semester, a teacher offering the course will do the continuous evaluation of the students at three points of time by conducting three tests of 20 marks each. Of these, two must be written tests and the third may be written test/quiz/ seminar/assignment for theoretical courses. Marks obtained in two best tests out of three will be awarded to the students. Each test will be of 1-hour duration based on unit or portion thereof taught in prescribed theory papers. A record of continuous evaluation should be maintained.
- (iii) The teacher offering the course will be responsible for setting the question paper and evaluating the answer books of tests and end semester examination of that course. In case of guest faculty involved in teaching or in case of other unavoidable circumstances, Head of the Department will make an alternate arrangement for the conduction of end term examination.
- (iv) Total of marks obtained in end semester examination and best of two tests under continuous evaluation will decide grade of the course.
- (v) The grading will be made on 10 point scale as described below:

| Letter Grade   | Grade points | Description   | Range of Marks |
|----------------|--------------|---------------|----------------|
| 0              | 10           | Outstanding   | 90-100         |
| A <sup>+</sup> | 9            | Excellent     | 80-89          |
| A              | 8            | Very good     | 70-79          |
| B <sup>+</sup> | 7            | Good          | 60-69          |
| В              | 6            | Above average | 50-59          |
| С              | 5            | Average       | 40-49          |
| Р              | 4            | Pass          | 35-39          |
| F              | 0            | Fail          | 0-34           |
| Ab             | 0            | Absent        | Absent         |

(vi) If a student obtains **F or Ab grade** in any course, he/she will be treated to have failed in the course. He/ she has to appear in the examination of the course as and when conducted/arranged by the University Teaching Department (UTD). Marks obtained earlier in continuous assessment may be carried forward and added to the marks obtained in the repeat end-term examination to decide the grade of the repeat course.

- (vii) The theoretical and practical courses can be repeated whenever offered or arrange by the Department but within maximum duration of the programme. **He/she can avail multiple repeat attempts to pass the course.**
- (viii) The Semester Grade Point Average (SGPA) and Cumulative Grade Point Average (CGPA) will be calculated as weighted average of **valid and virtual** credit points secured by the student . The SGPA and CGPA shall be rounded off up to 2 decimal place and shall be reported in the grade sheet.
- (ix) SGPA is measure of the performance of the student in a semester in a semester. It is a ratio of total credit points secured by a student in various courses registered in a semester and the total course credits taken during that semester, that is,

SGPA (S<sub>i</sub>)= 
$$\Sigma(C_i \times G_i)/\Sigma C_i$$
 =Total Credit points/Total credits

where  $C_i$  is the number of credits of the  $i^{th}$  course in a semester and  $G_i$  in the grade point scored by the student in the  $i^{th}$  course.

(x) CGPA is a measure of overall cumulative performance of a student over all the semesters completed. The CGPA is the ratio of total credit points secured by a student in various courses in all the semesters completed and some of the total credits of all courses in all the semesters completed.

$$CGPA = \Sigma(C_i \times S_i)/\Sigma C_i$$

Where S<sub>i</sub> is the SGPA of the i<sup>th</sup> semester and C<sub>i</sub> is the total number of credits in the i<sup>th</sup> semesters.

- (x) The dissertation / major project / internship report of 9 credit will be asseed by one external examiner to be appointed by the voice chancellor from the panel of examiner suggested by Head /Director and the supervising teacher /the examiner appointed by the Head /Director of the UTD.
- (xi) A comprehensive viva-voce of **4 virtual credits** will be conducted at the end of each semester of the programme by a board of four examiners, at least one of whom shall be external. The vice chancellor will appoint the external examiner in consultation with Head /Director of the UTD. Three will form a quorum. Head /director will coordinate the comprehensive viva-voce. The grade awarded in the viva-voce shall be shown separately in the grade sheet.
- (xii) If a programme has large number of students then more number of boards may be constituted as per requirement. The board may include at least two experts including one internal and one external.
- (xiii) On completing all requirements for award of the degree, the CGPA will be calculated and this value will be indicated on the degree along with division. The final degree will also indicate the division obtained as follows:
- **I Div. with distinction:** The candidate has earned minimum number of credits for the award of the degree in first attempt with CGPA of 8.00 or above.

**I Div.:** The candidate has earned minimum number of credits for the award of the degree in first attempt with CGPA of 6.50 or above but less than 8.00.

**II Div.:** The candidate has earned minimum number of credits for the award of the degree in first attempt with CGPA of 5.00 or above but less than 6.50.

**Pass Division:** The candidate has earned minimum number of credits for the award of the degree in first attempt with CGPA of 4.00 or above but less than 5.00.

- (xiv) The student will be promoted to the next semester if he/ she secured at least 12 valid credits in a semester. In case the student secure less than 12 valid credits in any semester, than the student will be asked to repeat the entire semester and the semester will be treated as zero semesters.
- (xv) Repetition of a theory practical course is allowed only to those candidates who get F or Ab in the course. The student has to pay the prescribed fee for repeating the course.
- (xvi) The guidelines issued by UGC time to time will be adopted for implementation.

| SEMESTER-I            |           |  |               |        |                  |
|-----------------------|-----------|--|---------------|--------|------------------|
| Course No.            | Paper No. | Title of the Paper (duration of examination) | Teaching Hrs. | Credit | End Semester+ CE |
| THEORY COURSES        |           |  |               |        |                  |
| Course 01(CHC101)     | Paper I   | Inorganic Chemistry (3 hours)                | 54            | 3      | 60+ 40 = 100     |
| Course 02 (CHC102)    | Paper II  | Organic Chemistry (3 hours)                  | 54            | 3      | 60+ 40 = 100     |
| Course 03 (CHC103)    | Paper III | Physical Chemistry (3 hours)                 | 54            | 3      | 60+ 40 = 100     |
| Course 04 (CHC104)    | Paper IV  | Spectroscopy (3 hours)                       | 54            | 3      | 60+ 40 = 100     |
| Course 05 (CHE101)    | Paper V   | CHE101A: Mathematics for Chemist (3 hours)   | 54            | 3      | 60+ 40 = 100     |
|                       | rapei v   | CHE101B: Biology for chemist (3 hours)       | 34            |        | 00+ 40 = 100     |
| PRACTICAL COURSES     |           |  |               |        |                  |
| Course 06 (CHC105)    |           | Practical Based on CHC101                    | 90            | 3      | 60+40 = 100      |
| Course oo (Cric 103)  |           | Inorganic Chemistry (6 Hrs; 1 day)           | 90            |        |                  |
| Course 07 (CHC106)    |           | Practical Based on CHC102                    | 90            | 3      | 60+40 = 100      |
| Course of (Cric 100)  |           | Organic Chemistry (6 Hrs; 1 day)             | 90            |        |                  |
| Course 08 (CHC107)    |           | Practical Based on CHC103                    | 90            | 3      | 60+40 = 100      |
| Codisc oo (Chicher)   |           | Physical Chemistry (6 Hrs; 1 day)            | 30            |        |                  |
| CHS101                |           | Skill Development                            |               | 2      | 100              |
| Total Marks, I SEM    |           | Total valid credits                          |               | 26     | 800              |
| Compressive Viva-voce |           |  |               | 4*     | 100              |

| SEMESTER II           |           |   |               |        |                  |
|-----------------------|-----------|---|---------------|--------|------------------|
| Course No.            | Paper No. | Title of the Paper (duration of examination)                    | Teaching Hrs. | Credit | End Semester+ CE |
| THEORY COURSES        | -         |   |               |        |                  |
| Course 01 (CHC-201)   | Paper I   | Inorganic Chemistry (3 hours)                                   | 54            | 3      | 60+ 40= 100      |
| Course 02 (CHC-202)   | Paper II  | Organic Chemistry (3 hours)                                     | 54            | 3      | 60+ 40 = 100     |
| Course 03 (CHC-203)   | Paper III | Physical Chemistry (3 hours)                                    | 54            | 3      | 60+ 40 = 100     |
| Course 04 (CHC-204)   | Paper IV  | Spectroscopy & Diffraction Methods (3 hours)                    | 54            | 3      | 60+ 40 = 100     |
| Course 04 (CHC-205)   | Paper V   | Computer for chemist (3 hours)                                  | 54            | 3      | 60+ 40 = 100     |
| PRACTICAL COURSE      |           |   |               |        |                  |
| Course 06 (CHC206)    |           | Practical Based on CHC201<br>Inorganic Chemistry (6 Hrs; 1 day) | 90            | 3      | 60+40 = 100      |
| Course 07 (CHC207)    |           | Practical Based on CHC202<br>Organic Chemistry (6 Hrs; 1 day)   | 90            | 3      | 60+40 =100       |
| Course 08 (CHC208)    |           | Practical Based on CHC203 Physical Chemistry (6 Hrs; 1 day)     | 90            | 3      | 60+40 = 100      |
| CHS201                |           | Skill Development   |               | 2      | 100              |
| Total Marks, II SEM   |           |   |               | 26     | 800              |
| Compressive Viva-voce |           |   |               | 4*     | 100              |

| SEMESTER III          |           |  |               |        | End Semester+ CE |
|-----------------------|-----------|--|---------------|--------|------------------|
| Course No.            | Paper No. | Title of the Paper (duration of examination)   | Teaching Hrs. | Credit | Max. Marks       |
| THEORY COURSES        |           |  |               |        |                  |
| Course 01(CHC301)     | Paper I   | Inorganic Chemistry (3 hours)  | 54            | 3      | 60+ 40 = 100     |
| Course 02 (CHC302)    | Paper II  | Organic Chemistry (3 hours)  | 54            | 3      | 60+ 40 = 100     |
| Course 03 (CHC303)    | Paper III | Physical Chemistry (3 hours)   | 54            | 3      | 60+ 40 = 100     |
| Course 04 (CHE301)    | Paper IV  | CHE301A: Molecular Dynamics CHE301B: Analytical Chemistry CHE301C: Photochemistry CHE301D: Biochemistry                        | 54            | 3      | 60+ 40 = 100     |
| Course 05 (CHE302)    | Paper V   | CHE302A: Theoretical Chemistry<br>CHE302B: Chemistry of Materials<br>CHE302C: Electrochemistry<br>CHE302D: Medicinal Chemistry | 54            | 3      | 60+ 40 = 100     |
| Course 06 (CHC304)    |           | Project report + Presentation  |               | 9      | 50+50=100        |
| CHS301                |           | Skill Development  |               | 2      | 100              |
| Total Marks, III SEM  |           |  |               | 26     | 700              |
| Compressive Viva-voce |           |  |               | 4*     | 100              |

| SEMESTER IV           |           |  |                  |        |                  |
|-----------------------|-----------|--|------------------|--------|------------------|
| Course No.            | Paper No. | Title of the Paper (duration of examination)   | Teaching<br>Hrs. | Credit | End Semester+ CE |
| THEORY COURSES        |           |  |                  |        |                  |
| Course 01 (CHC401)    | Paper I   | Inorganic Chemistry (3 hours)  | 54               | 3      | 60+ 40 = 100     |
| Course 02 (CHC402)    | Paper II  | Organic Chemistry (3 hours)  | 54               | 3      | 60+ 40 = 100     |
| Course 03 (CHC403)    | Paper III | Physical Chemistry (3 hours)   | 54               | 3      | 60+ 40 = 100     |
| Course 04 (CHE401)    | Paper IV  | Any one from 404A to 404D (3 hours) CHE401A: Organic Synthesis CHE401B: Polymers CHE401C: Organo Transitional Metal Chemistry CHE401D: Solid State Chemistry | 54               | 3      | 60+ 40 = 100     |
| Course 05 (CHE402)    | Paper V   | CHE402A: Chemistry of Natural Products CHE402B: Physical Organic Chemistry CHE402C: Environmental Chemistry CHE402D: Heterocyclic Chemistry                  | 54               | 3      | 60+ 40 = 100     |
| PRACTICAL COURSE      |           |  |                  |        |                  |
| Course 06 (CHC404)    |           | Practical Based on CHC401<br>Inorganic Chemistry (6 Hrs; 1 day)  | 90               | 3      | 60+40 = 100      |
| Course 07 (CHC405)    |           | Practical Based on CHC402<br>Organic Chemistry (6 Hrs; 1 day)  | 90               | 3      | 60+40 = 100      |
| Course 08 (CHC406)    |           | Practical Based on CHC403 Physical Chemistry (6 Hrs; 1 day)  | 90               | 3      | 60+40 = 100      |
| CHS401                |           | Skill Development  |                  | 2      | 100              |
| Total Marks, IV SEM   |           |  |                  | 26     | 900              |
| Compressive Viva-voce |           |  |                  | 4*     | 100              |
| Grand Total           |           |  |                  | 104    | 3400             |

<sup>\*</sup> Virtual Credit Continuous Evaluation (CE)

## M. Sc. I SEMESTER Course 01 (CHC-101) (PAPER I): Inorganic Chemistry

Maximum Marks: 100 (End Sem.:60+CE: 40)

Credit: 3 Teaching Hour: 54

#### **UNIT I**

Stereochemistry and Bonding in Main Group Compounds. VSEPR theory and its application for treating structures of inorganic molecules and ions containing lone pairs of electrons, shortcomings of VSEPR model. MO treatment of polyatomic molecules, e.g., ozone, nitrite, nitrate, hydarzoic acid and benzene. (11Hrs)

## **UNIT II**

Reaction Mechanism of Transition Metal Complexes. Inert and labile complexes, interpretation of lability and inertness of transition metal complexes on the basis of valence bond and crystal field theories. Kinetics of octahedral substitution: acid hydrolysis, factors affecting acid hydrolysis.

. (11Hrs)

#### **UNIT III**

Metal-Ligand Bonding . Molecular orbital theory. Qualitative aspects of metal-ligand  $\sigma$ -bonding in octahedral, tetrahedral and square planar complexes. Jahn-Teller Effect

Electronic Spectra and of Transition Metal Complexes. Spectroscopic term, terms and microstates for the  $p^2$  and  $d^2$  configurations, Hund's rules for ground state terms, the correlation of spectroscopic terms into Mulliken symbols, electronic transition selection rules, Orgel diagrams for transition metal complexes  $(d^1-d^9)$  states). Jahn-teller effect and electronic spectra of complexes.

(11Hrs)

#### **UNIT IV**

Metal  $\pi$ -Complexes. Metal carbonyls: structure and bonding, vibrational spectra of metal carbonyls for bonding and structural elucidation. Dioxygen complexes, Wilkinson's catalyst

(10Hrs)

## **UNIT V**

Borane Chemistry Metal Clusters. Bonding and topology of boranes, 4-digit coding (s, t, y, x) numbers for  $B_2H_6$ ,  $B_4H_{10}$ ,  $B_5H_{9}$ ,  $B_5H_{11}$  and  $B_6H_{10}$  and their utilities. Acquaintance with carboranes and metallocarboranes. Metal clusters: synthesis, reactivity and bonding.

(11Hrs)

- 1. Advanced Inorganic Chemistry, F.A. Cotton and Wilkinson, John Wiley.
- Inorganic Chemistry, J.E. Huhey, Harpes & Row.
- 3. Chemistry of the Elements. N.N. Greenwood and A. Earnshow, Pergamon.
- 4. Inorganic Electronic Spectroscopy, A.B.P. Lever, Elsevier.
- 5. Magnetiochemistry, R.1. Carlin, Springer Verlag.
- 6. Comprehensive Coordiantion Chemistry eds., G. Wilkinson, R.D. Gillars and J.A. McCleverty, Pergamon.

## M.Sc. SEMESTER I Course 02 (CHC-102) (PAPER II): Organic Chemistry

Maximum Marks: 100 (End Sem.:60+CE: 40) Credit: 3

**Teaching Hour: 54** 

#### **UNIT I**

Structure and Bonding. Bonding in organic molecules. Delocalized chemical bonding-conjugation, cross conjugation, Conjugation, resonance, hyperconjugation.

Aromaticity in benzenoid and non-benzenoid compounds, alternate and non-alternate hydrocarbons. Hűckel rule, anti-aromaticity, homo-aromaticity.

Bonds weaker than covalent bond. Hydrogen bonding, crown ether complexes, and cyclodextrins (11Hrs)

#### **UNIT II**

Stereochemistry. Chirality, elements of symmetry, molecules with more than one chiral center, threo and erythro isomers. R and S configuration. Separation of enantiomers. Regioselective, stereospecific and stereoselective rections. Asymmetric synthesis. Optical activity in the absence of chiral carbon (atropisomerism)-biphenyls, allenes and spiranes, and their nomenclature.

Conformational analysis of cyclohexanes and decalins. Effect of conformation on reactivity.

(11Hrs)

## **UNIT III**

Reaction Mechanism. Types of mechanisms, types of reactions, thermodynamic and kinetic requirements, and control, Potential energy diagrams, transition states and intermediates, methods of determining mechanisms, isotope effects.

Effect of structure on reactivity -resonance and field effects, steric effect. The Hammett equation and linear free energy relationship, substituent and reaction constants. Taft equation.

(10Hrs)

## **UNIT IV**

Aliphatic Nucleophilic Substitution. The  $S_N2$ ,  $S_N1$ , mixed  $S_N2$  and  $S_N1$ , and SET mechanisms. The  $S_Ni$  mechanism. Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium. The neighbouring group mechanism, neighbouring group participation by  $\pi$  and  $\sigma$  bonds. Classical and nonclassical carbocations, norbornyl system, carbocation rearrangements.

(10Hrs)

#### **UNIT V**

*Ultraviolet and Visible Spectroscopy.* Electromagnetic radiation, wavelength, wave number, frequency, and energy calculation. Electronic transitions (185-800 nm), Beer-Lambert law, effect of solvent on electronic transitions, Fieser-Woodward rules for conjugated dienes and carbonyl compounds.

Optical Rotatory Dispersion (ORD) and Circular Dichroism (CD). Concept of ORD and CD, deduction of absolute configuration, octant rule for ketones.

(12Hrs)

- 1. Organic Chemistry, J. Claden, N. Greeves, S. Warren, P. Wothers, Oxford University Press.
- Advanced Organic Chemistry-Reactions, Mechanism and Structure, Jerry March, Wiley-Interscience.
- 3. Organic Chemistry, P.Y. Bruice, Pearson Education Asia.
- 4. Organic Chemistry, L.G. Wade, Jr., Pearson Education.
- 5. Advanced Organic Chemistry, F. A. Carey and R. J. Sundberg, Plenum.
- 6. Organic Chemistry, J. McMurry, Thomson Asia.
- 7. Organic Chemistry, T.W.G. Solomons and C.B. Fryhle, John Wiley (Asia).
- 8. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman.
- 9. Organic Chemistry, R. T. Morrison and R. N. Boyd, Prentice-Hall.
- 10. Stereochemistry of Organic Compounds, E.L. Eliel and S.H. Wilen, John Wiley (Asia).
- 11. Stereochemistry of Organic Compounds, D. Nasipuri, New Age International.
- 12. Stereochemistry of Organic Compounds, P.S. Kalsi, New Age International.
- 13. Introduction to Spectroscopy, D.L. Pavia, G.M. Lampman and G.S. Kriz, Thomson, Brooks/Cole.
- Organic Spectroscopy, W. Kemp, ELBS, Macmillan.
- 15. Spectrometric Identification of Organic Compounds, R. M. Silverstein, G. C. Bassler and T. C, Morrill, John Wiley
- 16. Application of Spectroscopy of Organic Compounds, J. R. Dyer, Prentice Hall.
- 17. Spectroscopic Methods in Organic Chemistry, D. H. Williams, I. Fleming, Tata McGraw-Hili.

## M.Sc. I SEMESTER Course 03 (CHC-103) (PAPER III): Physical Chemistry

Maximum Marks: 100 (End Sem.:60+CE: 40) Credit: 3

Teaching Hour: 54

#### **UNIT I**

Introduction to exact quantum mechanical results. The Schrodinger equation and the postulates of quantum mechanics. Discussion of solutions of the Schrodinger equation to systems such as particle in a box, the harmonic oscillator, the rigid rotor, the hydrogen atom.

(11Hrs)

## **UNIT II**

Approximate Methods. The variation theorem, linear variation principle. Perturbation theory (introductory idea). Application of variation method to the Helium atom.

Angular Momentum. Ordinary angular momentum, generalized angular momentum, eigen functions for angular momentum, eigen values of angular momentum, addition of angular momenta, spin, antisymmetry and Pauli exclusion principle.

(12Hrs)

## **UNIT III**

Classical Thermodynamics. Brief resume of concepts of laws of thermodynamics, free energy, chemical potential and entropies. Partial molar properties; partial molar free energy, partial molar volume and partial molar heat content and their significance. Determinations of these quantities. Concept of fugacity and determination of fugacity.

Derivation of phase rule and its application to three component systems, second order phase transitions.

(11Hrs)

## **UNIT IV**

Chemical Dynamics (Part I). Methods of determining rate laws, Arrhenius equation, collision theory of reaction rates, steric factor, activated complex theory, ionic reactions, kinetic and thermodynamic control of reactions.

(10Hrs)

#### **UNIT V**

Chemical Dynamics (Part II). Dynamic chain (hydrogen-bromine reaction, pyrolysis of acetaldehyde, decomposition of ethane), photochemical (hydrogen-bromine and hydrogen-chlorine reactions) and oscillatory reactions, homogeneous catalysis, kinetics of enzyme reactions.

(10Hrs)

- Physical Chemistry, P.W. Atkins, ELBS.
- 2. Introduction to Quantum Chemistyry, A.K. Chandra, Tata Mc Graw Hill.
- 3. Quantum Chemistry, Ira N. Levine, Prentice Hall.
- 4. Coulson's Valence, R.Mc Ween y, ELBS.
- 5. Chemical Kinetics. K.J. Laidler, McGraw-Hill.
- 6. Kinetics and Mechanism of Chemical Transformation J.Rajaraman and J. Kuriacose, McMillan.
- 7. Micelles, Theoretical and Applied Aspects, V. MOraoi, Plenum.
- 8. Modern Electrochemistry Vol. 1 and Vol II J.O.M. Bockris and A.K.N. Reddy, Planum.
- 9. Introduction to Polymer Science, V.R. Gowarikar, N.V. Vishwanathan and J. Sridhar, Wiley Eastern.
- 10. Introduction to Quantum Chemistry-R.K. Prasad, New Age Publication.

## M.Sc. I SEMESTER Course 04 (CHC-104) (PAPER IV): Spectroscopy

Maximum Marks: 100 (End Sem.:60+CE: 40) Credit: 3

Teaching Hour: 54

## **UNIT I**

*Unifying Principles.* Electromagnetic radiation, interaction of electromagnetic radiation with matterabsorption, emission, transmission, reflection, refraction, dispersion, polarisation and scattering. Uncertainty relation and natural line width and natural line broadening, transition probability, transition moment, selection rules, intensity of spectral lines.

(11Hrs)

#### **UNIT II**

*Microwave Spectroscopy.* Classification of molecules, rigid rotor model, effect of isotopic substitution on the transition frequencies, intensities, non-rigid rotor. Stark effect, nuclear and electron spin interaction and effect of external field. Applications.

(10Hrs)

## **UNIT III**

Infrared Spectroscopy. Review of linear harmonic oscillator, vibrational energies of diatomic molecules, zero point energy, force constant and bond strengths; anharmonicity, Morse potential energy diagram, vibration-rotation spectroscopy, P,Q,R branches. Vibrations of polyatomic molecules. Selection rules, normal modes of vibration, group frequencies, overtones, hot bands, factors affecting the band positions and intensities, far IR region.

(12Hrs)

#### **UNIT IV**

Raman Spectroscopy. Classical and quantum theories of Raman effect. Pure rotational, vibrational and vibrational-rotational Raman spectra, selection rules, mutual exclusion principle. Resonance Raman spectroscopy, coherent anti Stokes Raman spectroscopy (CARS).

(10Hrs)

#### **UNIT V**

*Electronic Spectroscopy. Atomic Spectroscopy.* Energies of atomic orbitals, vector representation of momenta and vector coupling, spectra of hydrogen atom and alkali metal atoms.

*Molecular Spectroscopy.* Energy levels, molecular orbitals, vibronic transitions, vibrational progressions and geometry of the excited states, Franck-Condon principle, electronic spectra of polyatomic molecules. Emission spectra; radiative and non-radiative decay, internal conversion, charge-transfer spectra.

(11Hrs)

- Modern Spectroscopy, J.M. Hollas, John Wiley.
- 2. Applied Electron Spectroscopy for chemical analysis d. H. Windawi and F.L. Ho, Wiley Interscience.
- 3. NMR, NQR, EPr and Mossbauer Spectroscopy in Inorganic Chemistry, R.V. Parish, Ellis Harwood.
- 4. Physical Methods in Chemistry, R.S. Drago, Saunders College.
- Chemical Applications of Group Theory, F.A. Cotton.
- 6. Introduction to Molecular Spectroscopy, G.M. Barrow, Mc Graw Hill.
- 7. Basic Principles of Spectroscopy, R. Chang, Mc Graw Hill.
- 8. Theory and Application of UV Spectroscopy, H.H. Jaffe and M. Orchin, IBH Oxford.
- 9. Introduction to Photoelectron Spectroscopy, P.K. Ghosh, John Wiley.
- 10. Introduction to Magnetic Resonance. A Carrington and A.D. Maclachalan, Harper & Row.

## Course 05 (CHE-101A) (PAPER V): Mathematics for Chemists

(For students without Mathematics in B.Sc.)

Maximum Marks: 100 (End Sem.:60+CE: 40)

Credit: 3 Teaching Hour: 54

Unit I

Vectors. Vectors, dot, cross and triple products etc. gradient, divergence and curl, Vector Calculus.

Matrix Algebra. Addition and multiplication; inverse, adjoint and transpose of matrices.

(10Hrs)

#### Unit II

Differential Calculus. Functions, continuity and differentiability, rules for differentiation, applications of differential calculus including maxima and minima (examples related to maximally populated rotational energy levels, Bohr's radius and most probable velocity from Maxwell's distribution etc.).

(11Hrs)

**Unit III** 

*Integral calculus.* Basic rules for integration, integration by parts, partial fractions and substitution. Reduction formulae, applications of integral calculus. Functions of several variables, partial differentiation, co-ordinate transformations (e.g. Cartesian to spherical polar).

(11Hrs)

**Unit IV** 

Elementary Differential equations. First-order and first degree differential equations, homogenous, exact and linear equations. Applications to chemical kinetics, secular equilibria, quantum chemistry etc. second order differential equation and their solutions.

(11Hrs)

## Unit V

Permutation and Probability. Permutations and combinations, probability and probability theorems average, variance root means square deviation examples from the kinetic theory of gases etc., fitting (including least squares fit etc with a general polynomial fit.

(11Hrs)

- The chemistry Mathematics Book, E.Steiner, Oxford University Press.
- 2. Mathematics for chemistry, Doggett and Suiclific, Logman.
- 3. Mathematical for Physical chemistry : F. Daniels, Mc. Graw Hill.
- 4. Chemical Mathematics D.M. Hirst, Longman.
- 5. Applied Mathematics for Physical Chemistry, J.R. Barante, Prentice Hall.
- 6. Basic Mathematics for Chemists, Tebbutt, Wiley.
- 7. Mathematics for Chemists: Bhupendra Singh, Pragati Prakashan

## Course 05 (CHE-101B) (PAPER V): Biology for Chemists

(For students without Biology in B.Sc.)

Maximum Marks: 100 (End Sem.:60+CE: 40) Credit: 3

**Teaching Hour: 54** 

#### Unit I

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

(11Hrs)

Unit II

Carbohydrates. Conformation of monosaccharides, structure and functions of important derivatives of mono-saccharides like glycosides, deoxy sugars, myoinositol, amino sugars. Nacetylmuramic acid, sialic acid disaccharides and polysaccharides. Structural polysaccharides cellulose and chitin. Storage polysaccharides-starch and glycogen. Structure and biological function of glucosaminoglycans of mucopolysaccharides. Carbohydrates of glycoporteins and glycolipids. Role of sugars in biological recognition. Blood group substances. Ascorbic acid.

(11Hrs)

## **Unit III**

Lipid. Fatty acids, essential fatty acids, structure and function of triacylglycerols, glycerophospholipids, sphingolipids, cholesterol, bile acids, prostaglandins. Liproproteins-composition and function, role in atherosclerosis. Properties of lipid aggregates-micelles, bilayers, liposomes and their possible biological functions. Biological membranes. Fluid mosaic model of membrane structure. Lipid metabolism-boxidation of fatty acids.

(11Hrs)

### **Unit IV**

Amino-acids, Peptides and Proteins. Chemical and enzymatic hydrolysis of proteins to peptides, amino acid sequencing. Secondary structure of proteins. force responsible for holding of secondary structures. ahelix, -b-sheets, super secondary structure, triple helix structure of collagen. Tertiary structure of protein-folding and domina structure. Quaternary structure. Amino acid metabolism-degradation and biosynthesis of amino acids, sequence determination, chemical/enzymatic/mass spectral, racemization/detection. Chemistry of oxytocin and tryptophan releasing hormone (TRH).

(11Hrs)

#### Unit V

*Nucleic Acids.* Purine and pyrimidine bases of nucleic acids, base pairing via Hbounding. Structure of ribonucleic acids (RNA) and deoxyribonucleic acid (DNA), double helix model of DNA and forces responsible for holding it. Chemical and enzymatic hydrolysis of nucleic acids. The chemical basis for heredity, an overview of replication of DNA, transcription, translation and genetic code. Chemical synthesis of mono and trinucleoside.

(10Hrs)

- 1. Principles of Biochemistry, A.L. Lehninger, Worth Publishers.
- Biochemistry, L. Stryer, W.H. Freeman.
- 3. Biochemistry, J. David Rawan, Neil Patterson.
- 4. Biochemistry, Voet and Voet, John Wiley.
- 5. Outlines of Biochemistry E.E. Conn and P.K. Stumpf, John Wiley.

## PRACTICAL COURSES M.Sc. SEMESTER I

Emphasis should be placed on physical principles, reaction chemistry and the technique involved in experiments. Attention should be placed on stoichiometric calculations and statistical analysis of results. In regular classes, each student should perform all the experiments as selected by the Department from the list in the syllabus. In examination, students should be given different experiments or combination of experiments.

| Course | 06 (CHC105): Inorganic Chemistry (6 hours; 1 day) | End Sem. +CE<br>60+40=100 | Credit 3 |
|--------|---|---------------------------|----------|
|        | Viva voce + Record+ Attendance                    | 5+5+5=15                  |          |
|        | Two or three Experiments based on the following:  | 45                        |          |
| (a)    | Synthesis   |                           |          |
| (b)    | Quantitative analysis                             |                           |          |
| (c)    | Qualitative                                       |                           |          |
| (d)    | Spectral analysis of known compounds              |                           |          |

| (iii) Cour | rse 07 (CHC-106): Organic Chemistry (6 hours; 1 day) | End Sem. +CE<br>60+40=100 | Credit 3 |
|------------|--|---------------------------|----------|
|            | Viva voce + Record+ Attendance                       | 5+5+5=15                  |          |
|            | Two or three Experiments based on the following:     | 45                        |          |
| (a)        | Synthesis  |                           |          |
| (b)        | Quantitative analysis                                |                           |          |
| (c)        | Qualitative analysis                                 |                           |          |
| (d)        | Spectral analysis of known compounds                 |                           |          |

| (iii) Cours | (iii) Course 08 (CHC-107): Physical Chemistry (6 hours; 1 day) |          | Credit 3 |
|-------------|--|----------|----------|
|             | Viva voce + Record+ Attendance                                 | 5+5+5=15 |          |
|             | Two Experiments based on the following:                        | 45       |          |
| (a)         | Adsorption   |          |          |
| (b)         | Phase Equilibria   |          |          |
| (c)         | Solutions  |          |          |
|             |  |          |          |

| Compressive Viva voce | Max. Marks<br>100 | Credit 4* |
|-----------------------|-------------------|-----------|
|-----------------------|-------------------|-----------|

## Course 06 (CHC-105): Inorganic Chemistry

Qualitative and Quantitative Analysis

- a. Less common metal ions: Ti, Mo, w, Ti, Zr, Th, V, U (two metal ions in cationic/anionic forms).
- b. Insoluble- Oxides, sulphates and halides.
- c. Separation and determination of two metal ions Cu-Ni, Ni-Zn, Cu-Fe etc. Involving volumetric and gravimetric methods.

## Chromatography

Separation of cations and anions by Paper Chromatography

## Preparations

Preparation of selected inorganic compounds and their studies by measurements of decomposition temperature, molar conductance, IR and electronic spectra.

 $\begin{array}{lll} & & & & & & & & & & & & \\ [Zn(acac)_2\,(H_2O)_2] & & & & & & & \\ [Ni(acac)_2(H_2O)_2] & & & & & & \\ [Co(Meacac)_2(H_2O)_2] & & & & & \\ [Cu(Meacac)_2]_H_2O & & & & & \\ [Cu(Meacac)_2]_H_2O & & & & \\ \end{array}$ 

Interpretation of IR and Electronic Spectra of some known compounds

## Course 07 (CHC-106): Organic Chemistry

## Qualitative Analysis

Separation, purification and identification of compounds of binary mixture (one solid and one liquid/solid) using chemical separation and sublimation/distillation, etc. Their analysis by semi-micro chemical tests and spot tets. IR spectra to be used for functional group identification. Preparation of one derivative of each compound.

Emphasis should be placed on physical principles, reaction chemistry and the technique involved in analysis.

## Organic Synthesis

Purification of compounds by TLC and column chromatography.

Aromatic electrophilic sustitutions:

Synthesis of m-dinitrobenzene from nitrobenzene

Synthesis of 2,4-dinitro-1-chlorobenzene from chlorobenzene

Synthesis of 4-bromoaniline from acetanilide

#### Reduction reaction:

Synthesis of m-nitroaniline from m-dinitrobenzene

### Quantitative Analysis

Determination of the percentage or number of hydroxyl groups in an organic compound by acetylation method

Interpretation of IR and Electronic Spectra of some known compounds

#### Course 08 (CHC-107): Physical Chemistry

A list of experiments under different headings is given below. Typical experiments are to be selected from each type.

### Adsorption

To study surface tension -concentration relationship for solutions (Gibbs equation).

## Phase Equilibria

To construct the phase diagram for three component system (e.g., chloroform-acetic acid-water).

#### Chemical Kinetics

- Determination of the effect of (a) Change of temperature (b) Change of concentration of reactants and catalyst and (c) Ionic strength of the media on the velocity constant of hydrolysis of an ester/ionic reactions.
- (iv) Determination of the primary salt effect on the kinetics of ionic reactions and testing of the Bronsted relationship (iodide ion is oxidised by persulphate ion)

#### Solutions

- Determination of molecular weight of non-volatile and non-electrolyte/electrolyte by cryoscopic method and to determine the activity coefficient of an electrolyte.
- Enzyme kinetics -inversion of sucrose

- Vogel's Textbook of Quantitative Analysis, revised, J. Bassett, R. C. Denney, G. H. Jeffery and J. Mendham, ELBS.
- Analytical Chemistry, S.M. Khopkar, New Age International Ltd., New Delhi.
- 3. Synthesis and Characterization of Inorganic Compounds, W. L. Jolly, Prentice Hall
- Experiments and Techniques in Organic Chemistry, D. Pasto, C. Johnson and M. Miller, Prentice Hall
- Macroscale and Microscale Organic Experiments, K. L. Williamson, D. C. Heath.
- Systematic Qualitative Organic Analysis, H. Middleton, Adward Arnold 6.
- Handbook of Organic Analysis- Qualitative and Quantitative, H. Clarke, Adward Arnold.
- Vogel's Textbook of Practical Organic Chemistry, ELBS.
- F.G. Mann and B.C. Saunders, Practical Organic Chemistry, Orient Longman.
- 10.
- Findley's Practical Physical Chemistry, B. P. Levitt, Longman Experimental Physical Chemistry, R.C. Das and B. Behera, Tata McGraw Hill.
- Practical Physical Chemistry, A. M. James and F. E. Prichard, Longman 12.

## M.Sc. II SEMESTER Course 01 (CHC-201) (PAPER I): Inorganic Chemistry

Maximum Marks: 100 (End Sem.:60+CE: 40) Credit: 3

Teaching Hour: 54

#### Unit I

Metal-Ligand Equilibria in Solution. Stepwise and overall formation constants and their relationship, trends in stepwise constants, factors affecting the stability of metal complexes with reference to the nature of metal ion and ligand, chelate effect and its thermodynamic origin, determination of binary formation constants by Bierrum method , Job's and Mole ratio methods.

(10Hrs)

#### **UNIT II**

Reaction Mechanism of Transition Metal Complexes. Base hydrolysis, conjugate base mechanism, direct and indirect evidences in favour of conjugate mechanism. Substitution reactions in square planar complexes: The Trans effect and the *trans* influence: Polarization and  $\pi$ -Bonding theories, applications of Trans effect in synthesis, Kurnakove's test of distinguishing *cis* and *trans* isomers using the concept of trans effect, mechanism of substitution reactions in square planar complexes, factors affecting substitution reactions. Acquaintance of Trans effect in octahedral complexes

(12Hrs)

## **UNIT III**

*Metal-Ligand Bonding. Molecular orbital theory:* Qualitative aspect of metal-ligand  $\pi$ -bonding in octahedral complexes, tetrahedral and square planar complexes.

Electronic Spectra and Magnetic Properties of Transition Metal Complexes. Calculations of Dq, B and  $\beta$  parameters for Cr(III), Co(II) and Ni(II) complexes using electronic spectral data. Charge transfer spectra: ligand to metal and metal to ligand.

(11Hrs)

#### **UNIT IV**

 $Metal\pi$ -Complexes. Metal nitrosyls: Nitrosylating agents for synthesis of metal nitrosyls, vibrational spectra and x-ray diffraction studies of metal nitrosyls for bonding and structure elucidation, important reactions of transition metal nitrosyl complexes pertaining to potentiality in air pollution control, biomedical applications. Dinitrogen complexes, Vaska's compound.

(10Hrs)

## **UNIT V**

*Group Theory:* Symmetry elements and symmetry operations, symmetry groups or point groups, Schoenflies symbols, point group classifications, matrix representation of symmetry operations, group, necessary conditions for any set of elements to form a group, subgroups, classes in a group.

(11Hrs)

- 1. Advanced Inorganic Chemistry, F.A. Cotton and Wilkinson, John Wiley.
- 2. Inorganic Chemistry, J.E. Huhey, Harpes & Row.
- 3. Chemistry of the Elements, N.N. Greenwood and A. Earnshow, Pergamon.
- 4. Inorganic Electronic Spectroscopy, A.B.P. Lever, Elsevier.
- 5. Magnetochemistry, R.L. Carlin, Springer Verlag.
- 6. Comprehensive Coordination Chemistry eds., G. Wilkinson, R.D. Gillars and J.A. McCleverty, Pergamon.
- 7. Synthesis and characterization of some novel nitrosyl compounds, R. C. Maurya Pioneer Publications, Jabalpur, 2000.
- 8. Chemical Applications of Group Theory, F.A. Cotton, John Wiley.

## M.Sc. SEMESTER II Course 02 (CHC-202) (PAPER II): Organic Chemistry

Maximum Marks: 100 (End Sem.:60+CE: 40)

Credit: **Teaching Hour: 54** 

#### **UNIT I**

Aliphatic Electrophilic Substitution. Bimolecular mechanisms, S<sub>E</sub>2 and S<sub>E</sub>i mechanisms. The S<sub>E</sub>1 mechanism, electrophilic substitution accompanied by double bond shifts. Effect of substrates, leaving group and solvent polarity on the reactivity.

Aromatic Electrophilic Substitution. The arenium ion mechanism, orientation and reactivity. The ortho/para ratio, ipso attack. Vilsmeier reaction, Fries rearrangement.

(11Hrs)

#### **UNIT II**

Free Radicals. Free radical reactions and their stereochemistry.

Allylic halogenation (NBS), oxidation of aldehydes to carboxylic acids, hydroperoxide formation, replacement of diazonium group. Hunsdiecker reaction.

Electrons spin resonance (ESR) spectroscopy. Electron paramagnetism, derivative curves, q values and hyperfine splitting.

(11Hrs)

#### **UNIT III**

Addition to Carbon-Carbon Multiple Bonds. Mechanistic and stereochemical aspects of addition reactions. Hydroboration. Michael reaction. Sharpless asymmetric epoxidation.

Addition to Carbon-Hetero atom Multiple Bonds. Mechanism of metal hydride reduction of carbonyl compounds, acids, esters and nitriles. Wittig reaction.

Mechanism of condensation reactions involving enolates. Mannich, Benzoin, Perkin, and Stobbe reactions.

(11Hrs)

## **UNIT IV**

Aromatic Nucleophilic Substitution. The S<sub>N</sub>Ar, S<sub>N</sub>1, benzyne and S<sub>RN</sub>1 mechanisms. Reactivity, effect of substrate structure, leaving group and attacking nucleophile. Bucherer reaction, alkylation, and amination. The Bamberger rearrangement. The von Richter rearrangement.

(10Hrs)

## **UNIT V**

Infrared and Raman Spectroscopy. Instrumentation and sample handling. Calculation of vibrational frequencies. Characteristic vibrational frequencies of alkanes, alkynes, carbonyl compounds, alcohols, ethers, amines, phenols and aromatic compounds. Finger-print region. Effect of hydrogen bonding and solvent effect on vibrational frequencies, overtones, combination bands and Fermi resonance. FT-IR.

Resonance Raman effect. Concept and factors that influence group frequencies.

(11Hrs)

- Organic Chemistry, J. Claden, N. Greeves, S. Warren, P. Wothers, Oxford University Press.
- Advanced Organic Chemistry-Reactions, Mechanism and Structure, Jerry March, Wiley-Interscience.
- 3. Organic Chemistry, P.Y. Bruice, Pearson Education Asia.
- Advanced Organic Chemistry, F. A. Carey and R. J. Sundberg, Plenum.
- 5. Organic Chemistry, J. McMurry, Thomson Asia.
- Organic Chemistry, T.W.G. Solomons and C.B. Fryhle, John Wiley (Asia).
- 7. Organic Chemistry, L.G. Wade, Jr., Pearson Education.
- A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman. 8.
- 9.
- Organic Chemistry, R. T. Morrison and R. N. Boyd, Prentice-Hall.
  Stereochemistry of Organic Compounds, E.L. Eliel and S.H. Wilen, John Wiley (Asia). 10.
- Stereochemistry of Organic Compounds, D. Nasipuri, New Age International. 11. Stereochemistry of Organic Compounds, P.S. Kalsi, New Age International. 12.
- Introduction to Spectroscopy, D.L. Pavia, G.M. Lampman and G.S. Kriz, Thomson, Brooks/Cole. 13.
- Organic Spectroscopy, W. Kemp, ELBS, Macmillan. 14.
- Spectrometric Identification of Organic Compounds, R. M. Silverstein, G. C. Bassler and T. C, Morrill, John Wiley 15.
- Application of Spectroscopy of Organic Compounds, J. R. Dyer, Prentice Hall. 16.
- Spectroscopic Methods in Organic Chemistry, D. H. Williams, I. Fleming, Tata McGraw-Hili. 17.

## M.Sc. II SEMESTER Course 03 (CHC-203) (PAPER III): Physical Chemistry

Maximum Marks: 100 (End Sem.:60+CE: 40) Credit: 3

**Teaching Hour: 54** 

#### **UNIT I**

Chemical Dynamics (Part III). General features of fast reactions, study of fast reactions by flow method, relaxation method, flash photolysis and the nuclear magnetic resonance method. Dynamics of molecular motions and of barrierless chemical reactions in solution, probing the transition state. Dynamics of unimolecular reactions; Lindemann-Hinshelwood and Rice-Ramsperger-Kassel-Marcus and Slater theories of unimolecular reactions.

(11Hrs)

#### **UNIT II**

Adsorption. Surface tension, capillary action, pressure difference across curved surface, Laplace equation, vapour pressure of droplets, Kelvin equation; Gibbs adsorption isotherm. Multilayer adsorption, BET equation. Calculation of surface area, catalytic activity at surfaces.

Surface films on liquids; electrokinetic phenomena; surface active agents. Micellisation, hydrophobic interaction. Critical micellar concentration. Solubilisation. Donnan's membrane equilibria.

(11Hrs)

## **UNIT III**

*Electrochemistry of solutions.* Debye-Huckel -Onsager treatment and its extension to concentrated solutions. Ion size factor and ion-solvent interactions. Concept of activity. Determination of mean ionic activity and activity coefficient.

Lippmannn electrocapillary phenomenon. Electrocapillary curves of mercury and their interpretation. Structure of electrified interfaces. Helmholtz, Guoy and Chapmann and Stern models. Introductory idea of advancements in electrified surfaces. Electrokinetic potential, its determination and significance.

(11Hrs)

## **UNIT IV**

*Macromolecules and Colloids.* Polymers, types of polymers, kinetics of polymerization, mechanism of polymerization reactions. Molecular mass of macromolecues, number and mass average molecular mass; molecular mass determination (osmometry, viscometry, diffusion and light scattering methods), sedimentation, chain structures and their configuration.

Emulsions. Theories of emulsification, coagulation, slow and rapid coagulation. Kenitics of coagulation. Von Smoluchouski equation and its verification.

(11Hrs)

#### **UNIT V**

*Irreversible electrode phenomenon.* Decomposition voltage and overvoltage. Consecutive electrode processes. Exchange current density. Butler-Volmer's equation. Tafel's plot. Theory of polarography. Ilkovic equation. Half wave potential and its significance.

Introduction to corrosion. Forms of corrosion. Corrosion monitoring and prevention.

(10Hrs)

- Physical Chemistry, P. W. Atkins, ELBS. .
- 2. Introduction to Quantum Chemistry, A.K. Chandra, Tata McGraw Hill.
- 3. Quantum Chemistry, Ira N. Levine, Prentce Hall.
- 4. Coulson's Valence, R. McWeeny, ELBS.
- Chemical Kinetics, K. J. Laidler, Mcgraw-Hill.
- 6. Kinetics and Mechanism of Chemical Transformations, J. Rajaraman and J. Kurjacose, McMillan,
- Micelles, Theoretical and Applied Aspects, V. Moroi, Plentm
- 8. Modern Electrochemistry Vol. I and Vol. II, J.O.M. Bockris and A.K.N. Reddy, Plenum.
- 9. Introduction to Polymer Science, V.R. Gowarikar, N.V. Vishwanathan and J. Sridhar, Wiley Eastern.
- 10. Physical Chemistry, W.J. Moore, Prentice-Hall, India.
- 11. Physical Chemistry, P.C. Rakshit.
- 12. Quantum Chemistry, Eyring and Kimball.

## M.Sc. II SEMESTER Course 04 (CHC-204) (PAPER IV): Spectroscopy & Diffraction Methods

Maximum Marks: 100 (End Sem.:60+CE: 40) Credit: 3

**Teaching Hour: 54** 

#### **UNIT I**

Photoelectron Spectroscopy. Basic principles; photo-electric effect, ionization process, Koopman's theorem. Photoelectron spectra of simple molecules, ESCA, chemical information from ESCA. Auger electron spectroscopy -basic idea.

*Photoacoustic Spectroscopy.* Basic principles of photoacoustic spectroscopy (PAS), chemical and surface applications.

(11Hrs)

#### **UNIT II**

*X-ray Diffraction.* Bragg condition, Miller indices, Laue method, Bragg method, Debye-Scherrer method of X-ray structural analysis of crystals, index reflections, identification of unit cells from systematic absences in diffraction pattern. Structure of simple lattices and X-ray intensities, structure factor and its relation to intensity and electron density. Description of the procedure for an X-ray structure analysis.

(11Hrs)

## **UNIT III**

*Electron Diffraction.* Scattering intensity vs. scattering angle, Wierl equation, measurement technique, elucidation of structure of simple gas phase molecules. Low energy electron diffraction and structure of surfaces.

*Neutron Diffraction.* Scattering of neutrons by solids and liquids, magnetic scattering, measurement techniques. Elucidation of structure of magnetically ordered unit cell.

(10Hrs)

#### **UNIT IV**

*Biological Cell and its Constituents.* Biological cell. Structure and functions of proteins, enzymes, DNA and RNA in living systems. Helix coil transition.

*Bioenergetics*. Standard free energy change in biochemical reactions; exergonic and endergonic reactions. Hydrolysis of ATP. Synthesis of ATP from ADP.

Statistical Mechanics in Biopolymers. Chain configuration of macromolecules, statistical distribution end to end dimensions. Polypeptide chain binding and proteins, introduction to protein folding problem.

(12Hrs)

## **UNIT V**

Thermodynamics of Biopolymer Solutions. Thermodynamics of biopolymer solutions, osmotic pressure, membrane equilibrium.

Transport of Ions. Biopolymers and their molecular weights. Structure and functions of cell membrane, ion transport through cell membrane, Nerve conduction; Evaluation of size, shape and molecular weight of biopolymers by various experimental techniques.

(10Hrs)

- Modern Spectroscopy, J.M. Hollas, John Wiley.
- 2. Applied Electron Spectroscopy for Chemical Analysis Ed. H. Windawi and F.L. Ho, Wiley Interscience.
- 3. Physical Methods in Chemistry, R.S. Drago, Saunders College.
- 4. Introduction to Molecular Spectroscopy, G.M. Barrow, McGraw Hill.
- 5. Basic Principles of Spectroscopy, R. Chang, McGraw Hill.
- 6. Introduction to Photoelectron Spectroscopy: P. K. Ghosh, John Wiley.
- 7. Principles of Biochemistry, A. L. Lehninger, Worth Publishers.
- Biochemistry, L.Stryer, W.H.Freeman.
- 9. Biochemistry, J. David Rawn, Neil Patterson.
- 10. Biochemistry, Voet and Voet, John Wiley.
- 11. Outlines of Biochemistry, E. E. Conn and P. K. Stumpf, John Wiley.
- 12. Bioorganic Chemistry: A Chemical Approach to Enzyme Action, H. Dugas and C. Penny, Springer-Verlag.
- 13. Macromolecules: Structure and Function, F. Wold, Prentice Hall.
- 14. Fundamentals of molecular spectroscopy, C.N. Banwell, Tata McGraw-Hill, New Delhi.
- 15. Instrumental Methods of Analysis, Willard, Meritt and Dean.

## Course 05 (CHC-205): (PAPER V): Computers for Chemists

This is a theory cum-laboratory course with more emphasis on laboratory work.

Maximum Marks: 100 (End Sem.:60+CE: 40)

Credit: 3 Teaching Hour: 54

#### Unit I

Introduction to Computers and Computing. Basic structure and functioning of computer with a PC as illustrative example. Memory I/O devices. Secondary storage Computer languages. Operating systems with DOS as an example Introduction to UNIX and WINDOWS. Principles of programming Alogrithms and flow-charts.

(10Hrs)

#### Unit II

Computer Programming in FORTRAN/C/BASIC. (the language features are listed here with reference to FORTRAN. The instructor may choose another language such as BASIC or C the features may be replaced appropriately). Elements of the compute language. Constants and variables. Operations and symbols Expressions. Arithmetic assignment statement. Input and output Format statement. Termination statements. Branching statements as IF or GO TO statement. LOGICAL variables. Double precession variables. Subscripted variables and DIMENSION. DO statement FUNCTION AND SUBROUTINE. COMMON and DATA statement (Student learn the programming logic and these language feature by hands on experience on a personal computer from the beginning of this topic.)

(12Hrs)

## **Unit III**

Programming in Chemistry. Developing of small computer codes using any one of the languages FORTRAN/C/BASIC involving simple formulae in Chemistry, such as Van der Waals equation. Chemical kinetics (determination of Rate constant) Radioactive decay (Half Life and Average Life). Determination Normality, Molarity nd Molality of solutions. Evaluation Electronegativity of atom and Lattice Energy from experimental determination of molecular weight and percentage of element organic compounds using data from experimental metal representation of molecules in terms of elementary structural features such as bond lengths, bond angles.

(12Hrs)

## **Unit IV**

Use of Computer programmes. Operation of PC. Data Processing. Running of standard Programs and Packages such as MS WORD, MS EXCEL -special emphasis on calculations and chart formations. X-Y plot. Simpson's Numerical Integration method. Programmes with data preferably from physical chemistry laboratory.

(10Hrs)

## Unit V

*Internet.* Application of Internet for Chemistry with search engines, various types of files like PDF, JPG, RTF and Bitmap. Scanning, OMR, Web camera.

- 1. Fundamentals of Computer: V. Rajaraman, Prentice Hall.
- 2. Computers in Chemistry: K.V. Raman, Tata Mc Graw Hill).
- 3. Computer Programming in FORTRAN IV-V Rajaraman, Prentice Hall.
- 4. Computers and Common Sense, R. Hunt and J. Shelley, Prentice Hall.
- 5. Computational Chemistry, A.C. Norris.
- 6. Microcomputer Quantum Mechanics, J.P. Killngbeck, Adam Hilger.
- 7. An Introduction to Digital Computer Design, V. Rajaraman and T. Radhakrishnan, Prentice Hall.

## M.Sc. SEMESTER II LABORATORY COURSE CHC 06-08 (CHC 206, CHC 207 and CHC 208)

Emphasis should be placed on physical principles, reaction chemistry and the technique involved in experiments. Attention should be placed on stoichiometric calculations and statistical analysis of results. In regular classes, each student should perform all the experiments as selected by the Department from the list in the syllabus. In examination, students should be given different experiments or combination of experiments.

| Course | 06 (CHC-206): Inorganic Chemistry (6 hours; 1 day) | End Sem. +CE<br>60+40=100 | Credit 3 |
|--------|--|---------------------------|----------|
|        | Record +Viva voce + Attendance                     | 5+5+5=15                  |          |
|        | Two or three Experiments based on the following    | 45                        |          |
| (a)    | Chromatographic separation                         |                           |          |
| (b)    | Synthesis  |                           |          |
| (c)    | Spectral analysis of known compounds               |                           |          |
|        |  |                           |          |

| (iii) Cou | rse 07(CHC-207): Organic Chemistry (6 hours; 1 day) | End Sem. +CE<br>60+40=100 | Credit 3 |
|-----------|---|---------------------------|----------|
|           | Record +Viva voce + Attendance                      | 5+5+5=15                  |          |
|           | Two or three Experiments based on the following:    | 45                        |          |
| (a)       | Synthesis   |                           |          |
| (b)       | Quantitative analysis                               |                           |          |
| (c)       | Spectral analysis of known compounds                |                           |          |
|           |   | ·                         |          |

| (iii) Course | e 08 (CHC-208): Physical Chemistry (6 hours; 1 day) | End Sem. +CE<br>60+40=100 | Credit 3 |
|--------------|---|---------------------------|----------|
|              | Record +Viva voce + Attendance                      | 5+5+5=15                  |          |
|              | Two Experiments based on the following:             | 45                        |          |
| (a)          | Electrochemistry                                    |                           |          |
| (b)          | Potentiometry                                       |                           |          |
| (c)          | Polarimetry   |                           |          |
|              |   |                           |          |

| Compressive Viva voce | Max. Marks 100 | Credit 4* |
|-----------------------|----------------|-----------|

## Course 06 (CHC-206): Inorganic Chemistry

Chromatography Separation of cations and anions by Column Chromatography; Ion exchange.

#### **Preparations**

Preparation of selected inorganic compounds and their studies by measurements of decomposition temperature, molar conductance, I.R., electronic spectra, and magnetic susceptibility measurements.

- 1. [Co(NH3)6] [Co(NO2)<sub>6</sub>]
- 2. cis-[Co(trien) (NO2)<sub>2</sub>]CI.H<sub>2</sub>O
- 3. Hg[Co(SCN)<sub>4</sub>]
- 4. [Co(Py)2Cl2]
- 5. [Ni(NH3)<sub>6</sub>]Cl2
- 6. [Ni(dmg)<sub>2</sub>]
- 7. [Cu(NH<sub>3</sub>)<sub>4</sub>]SO<sub>4</sub> H<sub>2</sub>O

Interpretation of TG and NMR spectra of some known compounds

## Course 07 (CHC-207): Organic Chemistry

Organic Synthesis

Oxidation reaction:

Synthesis of 9,10-anthraquinone by oxidation of anthracene by chromium trioxide

Synthesis of 4-nitrobenzaldehyde by oxidation of 4-nitrotoluene by chromium trioxide

Cannizzaro reaction

Synthesis of benzyl alcohol from benzaldehyde

Claisen-Schmidt reaction:

Synthesis of dibenzylideneacetone (1,5-diphenylpenta-1,4-dien-3-one) from acetone and benzaldehyde

### Sandmeyer reaction:

Synthesis of 2-chloroanthranilic acid from anthranilic acid

### Methylation:

Synthesis of methyl 2-naphthyl ether (2-methoxynaphthalene, nerolin) by methylation of 2-naphthol by dimethyl sulphate.

#### Quantitative Analysis

Determination of the percentage or number of hydroxyl groups in an organic compound by acetylation

Determination of aromatic amines or phenols using bromate-bromide mixture

Determination of number of double bonds in an organic compound

Determination of percentage or number of ester groups in an organic compound by saponification

Interpretation of NMR and mass spectra of some known compounds

## Course 08 (CHC-208): Physical Chemistry

A list of experiments under different headings is given below. Typical experiments are to be selected from each type.

#### Electrochemistry

#### A. Conductometry

- Determination of the velocity constant, order of the reaction and energy of activation for saponification of ethyl acetate by sodium hydroxide conductometrically.
- Determination of solubility and solubility product of sparingly soluble salts (e.g., PbSO<sub>4</sub>, BaSO<sub>4</sub>) (ii) conductometrically.
- (iii) Determination of the strength of strong and weak acids in a given mixtureconductometrically.
- (iv) Determination of the activity coefficient of zinc ions in the solution of 0.002 M zinc sulphate using Debye-Huckel's limiting law.

## B. Potentiometry/pH merry

- Determination of strengths of halides in a mixture potentiometrically.
- (ii) Determination of the valency of mercurous ions potentiometrically.
- (iii) Determination of the strength of strong and weak acids in a given mixture usi potentiometer/pH meter.
- Determination of activity and activity coefficient of electrolytes. (iv)

#### Polarimetry

- Determination of rate constant for hydrolysis/inversion of sugar using a polarimeter.
- (ii) Enzyme kinetics -inversion of sucrose

- Vogel's Textbook of Quantitative Analysis, revised, J. Bassett, R. C. Denney, G. H. Jeffery and J. Mendham, ELBS. 1.
- Analytical Chemistry, S.M. Khopkar, New Age International Ltd., New Delhi. 2.
- 3. Synthesis and Characterization of Inorganic Compounds, W. L. Jolly, Prentice Hall
- Experiments and Techniques in Organic Chemistry, D. Pasto, C. Johnson and M. Miller, Prentice Hall 4.
- 5. Macroscale and Microscale Organic Experiments, K. L. Williamson, D. C. Heath.
- Systematic Qualitative Organic Analysis, H. Middleton, Adward Arnold. 6.
- Handbook of Organic Analysis- Qualitative and Quantitative, H. Clarke, Adward Arnold.
- Vogel's Textbook of Practical Organic Chemistry, ELBS.
- F.G. Mann and B.C. Saunders, Practical Organic Chemistry, Orient Longman.
- Findley's Practical Physical Chemistry, B. P. Levitt, Longman Experimental Physical Chemistry, R.C. Das and B. Behera, Tata McGraw Hill.
- Practical Physical Chemistry, A. M. James and F. E. Prichard, Longman

## M.Sc. SEMESTER III Course 01 (CHC-301) (PAPER I): Inorganic Chemistry

Maximum Marks: 100 (End sem.:60+CE:40)

Credit: 3 Teaching Hour: 54

#### **UNIT I**

*Group theory.* Matrix representation of point groups, Character of a representation, reducible and irreducible representations. The great orthogonality theorem (without proof) and its importance, construction of character tables for  $C_{2v}$ , and  $C_{3v}$  point groups, importance of character tables.

(12Hrs)

## **UNIT II**

Group theory and vibrational Spectroscopy. Group theory to symmetry, shapes and molecular energy level diagrams of molecules like BF<sub>3</sub>, NH<sub>3</sub> (AB<sub>3</sub> type),  $[Pt(NH_3)_4]^{2^+}$ ,  $[Ni(CN)_4]^{2^-}$  (AB<sub>4</sub> type) and  $[Co(NH_3)_6]^{3^+}$  (AB<sub>6</sub> type) molecules. Modes of bonding of ligands such as SCN<sup>-</sup>,  $\beta$ -ketoenolate and related ligands, nitrate ion and corboxylates.

(12Hrs)

#### **UNIT III**

*Nuclear Magnetic Resonance Spectroscopy.* NMR Shift reagents, shift mechanism and its utility in simplification of NMR spectra. Applications of NMR in characterization of coordination compounds.

(10Hrs)

## **UNIT IV**

Bioinorganic Chemistry. Metal containing enzymes: Carboxypeptidase-A, Carbonic anhydrase, arginase, urease, DNA polymerase, phosphoglucomutase (glucose storage): structure and reactivity

(10Hrs)

## **UNIT V**

*Transport and Storage of Dioxygen:* structure and function of hemoglobin, myoglobin, hemocyanins and hemorythrin. Poisoning towards hemoglobin and myoglobin.

(10Hrs)

- 1. Chemical Applications of Group Theory, F.A. Cotton, John Wiley
- 2. Physical Methods for Chemistry, R.S. Drago, Saunders Compnay.
- 3. Structural Methods in Inorganic Chemistry, E.A.V. Ebsworth, D.W.H. Rankin and S. Cradock, ELBS.
- 4. Infrared and Raman Spectral: Inorganic and Coordination Compounds K. Nakamoto, Wiley.
- 5. Progress in Inorganic Chemistry vol., 8, ed., F.A. Cotton, vol., 15 ed. S.J. Lippard, Wiley.
- 6. Transition Metal Chemistry ed. R.L. Carlin vol. 3 dekker.
- 7. Inorganic Electronic Spectroscopy, A.P.B. Lever, Elsevier.
- 8. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, .V. Parish, Ellis Haywood.
- 9. Practical NMR Spectroscopy, M.L. Martin. J.J. Deepish and G.J. Martin, Heyden.
- 10. Introduction to NMR spectroscopy, R.J. Abraham, J. Fisher and P. Loftus, Wiley.
- 11. Spectroscopic Methods in Organic Chemistry D.H. Williams, I. Fleming, Tata McGraw-Hill.

## M.Sc. SEMESTER III Course 02 (CHC-302) (PAPER II): Organic Chemistry

Maximum Marks: 100 (End Sem.:60+CE: 40) Credit: 3

**Teaching Hour: 54** 

#### **UNIT I**

Nuclear Magnetic Resonance Spectroscopy. <sup>1</sup>H-NMR phenomenon. chemical shift, shielding and deshielding mechanism, mechanism of measurement, chemical shift values and its correlation for protons bonded to carbon (aliphatic, olefinic, aldehydic and aromatic) and other nuclei (alcohols, phenols, enols, carboxylic acids, amines, amides and mercapto). Chemical exchange, effect of deuteration. Spin-spin coupling (first order spectra; AX, AB, AMX spectra). Coupling constant, Karplus curve. Complex spin-spin interactions. Simplification of complex spectra, nuclear magnetic double resonance, increased field strength, contact shift reagents. Nuclear Overhauser effect (NOE). FT technique.

(12Hrs)

#### **UNIT II**

Photochemistry: Part I. Photochemical Reactions. Interaction of electromagnetic radiation with matter, types of excitations, fate of excited molecule, quantum yield.

Photochemistry of Carbonyl Compounds. Norrish type I and type II reactions;  $\alpha$ -cleavage of cyclic and acyclic,  $\beta,\gamma$ - unsaturated and  $\alpha,\beta$ -unsaturated compounds. Dimerisation, and the Patterno-Büchi reaction. Rearrangement of dienones. Photoreduction.

(11Hrs)

#### **UNIT III**

*Photochemistry: Part II.* Photochemistry of Alkenes. Geometrical isomerisation, dimerisation reactions, rearrangement of 1,4- and 1,5- dienes. Photooxidation.

Photochemistry of Aromatic Compounds. Photo-Fries rearrangement, photoisomerization. Barton reaction. Singlet molecular oxygen reactions.

(10Hrs)

#### **UNIT IV**

Pericyclic Reactions: Part I. Molecular orbitals and their symmetry. Molecular orbitals of ethylene, 1,3- butadiene, 1,3,5-hexatriene and allyl system, and their symmetry properties.

Pericyclic reactions. Characteristics and classification. Electrocyclic reactions: conrotatory and disrotatory motions, 4n, 4n+2 and allyl systems. Woodward-Hoffmann correlation diagrams. FMO and PMO approach.

(10Hrs)

#### **UNIT V**

Pericyclic Reactions: Part II. Cycloaddditions. Woodward-Hoffmann correlation diagrams. FMO and PMO approach. Antarafacial and suprafacial additions. 4n and 4n+2 systems, 2+2 addition of ketenes. Ene synthesis.

Sigmatropic Rearrangements. Suprafacial and antarafacial 1,3- and 1,5- shifts of H, sigmatropic shifts involving carbon moieties, 2,3-, and 3,3-sigmatropic rearrangements. Claisen, Cope, aza-Cope, Sommlet-Hauser, and Fisher Indole rearrangements.

(11Hrs)

- 1. Essentials of Molecular Photochemistry, A Gilbert and J. Baggott, Blackwell Scientific Publication.
- 2. Molecular Photochemistry, N.J. Turro, W.A. Benjamin.
- 3. Introductory Photochemistry, A. Cox and t. Camp, McGraw Hill.
- 4. Photochemistry, R.P. Kundall and A. Gilbert. Thomson Nelson.
- 5. Organic Photochemistry, J. Coxon and B.halton, Cambridge University Press.
- 6. Introduction to Spectroscopy, D.L. Pavia, G.M. Lampman and G.S. Kriz, Thomson, Brooks/Cole.
- Spectroscopic Methods in Organic Chemistry D.H. Williams, I. Fleming, Tata McGraw-Hill.
- 8. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, .V. Parish, Ellis Haywood.
- 9. Spectrometric Identification of Organic Compounds, R.M. Silverstein, G.C. Bassler adn T.C. Morrill, John Wiley.
- 10. Application of Spectroscopy of Organic Compounds, J.R. Dyer Prentice Hall.
- 11. Pericyclic Reactions, S. M. Mukherji, Macmillan, India.
- 12. Organic Chemistry, L.G. Wade, Jr., Pearson Education.
- 13. Advanced Organic Chemistry-Reactions, Mechanism and Structure, Jerry March, Wiley-Interscience.

## M.Sc. SEMESTER III Course 03 (CHC-303) (PAPER III): Physical/Solid State Chemistry

Maximum Marks: 100 (End Sem.:60+CE: 40) Credit: 3

Teaching Hour: 54

#### **UNIT I**

*Electronic Structure of Atoms.* Electronic configuration, Russell-Saunders terms and coupling scheme, Slater parameters, magnetic effects. Zeeman splitting; virial theorem.

(10Hrs)

#### **UNIT II**

Molecular Orbital Theory. Hückel theory of conjugated systems, bond order and charge density calculations. Applications to ethylene, butadiene, and cyclobutadiene. Introduction to extended Hückel theory.

(10Hrs)

#### **UNIT III**

Homogeneous Catalysis. Stoichiometric reactions for catalysis, homogeneous catalytic hydrogenation, Zeigler-Natta polymerisation of olefins.

Heterogenous Catalysis. Thermodynamics of active centres, mechanism of heterogenous catalysis; structural promotion and structural modification.

(11Hrs)

## **UNIT IV**

*Crystal Defects.* Perfect and imperfect crystals, stoichiometric and non-stoichiometric defects. Intrinsic and extrinsic defects, point defects, line and plane defects; Schottky and Frenkel defects.

*Solid State Reactions.* General principles, coprecipitation as a precursor to solid state reactions, factors affecting solid state reactions.

(12Hrs)

#### **UNIT V**

*Electronic Properties and Band Theory.* Metals, insulators and semiconductors. Electronic structure of solids-Band theory; band structure of metals, insulators and semiconductors. Intrinsic and extrinsic semiconductors, doping semiconductors, p-n junctions, superconductors.

(11Hrs)

- 1. Solid state chemistry and its applications, A.R. West. Peenum.
- 2. Principles of the Solid State, H.V. Keer, Wiley Eastern.
- 3. Solid State Chemistry, N.B. Hannay.
- 4. Solid State Chemistry, D.K. Chakrabarty, New Wiley Eastern.

## M.Sc. SEMESTER III Course 04 (CHE-301A) (ELECTIVE PAPER IV): Molecular Dynamics

Maximum Marks: 100 (End Sem.:60+CE: 40) Credit: 3

Teaching Hour: 54

#### **UNIT I**

*Principles of Reactivity.* Mechanistic significance of entropy, enthalpy and Gibb's free energy. Arrhenius equation. Transition state theory. Uses of activation parameters, Hammond's postulate. Bell-Evans-Polanyi principle. Potential energy surface model. Marcus theory of electron transfer. Reactivity and selectivity principles.

(10Hrs)

#### **UNIT II**

*Kinetic Isotope Effect.* Theory of isotope effects. Primary and secondary kinetic isotope effects. Heavy atom isotope effects. Tunneling effect. Solvent effects.

(10Hrs)

#### **UNIT III**

Structural Effects on Reactivity. Linear free energy relationships (LFER). The Hammett equation, substituent constants, theories of substituent effects. Interpretation of  $\sigma$ -values. Reaction constant  $\rho$ . Deviations from Hammett equation. Dual-parameter correlations, inductive substituent constant. The Taft model,  $\sigma_{\text{I}}$ - and  $\sigma_{\text{R}}$ -scales.

(10Hrs)

#### **UNIT IV**

Solvation and Solvent Effects. Quantitative understanding of solvent-solute effects on reactivity. Thermodynamic measure of solvation. Effects of solvation on reaction rates and equilibria. Various empirical indices of solvation based on physical properties, solvent-sensitive reaction rates, spectroscopic properties and scales for specific solvation. Use of solvation scales in mechanistic studies. Solvent effects from the curve-crossing model.

(12Hrs)

## **UNIT V**

- (a) Pharmacokinetics. Introduction to drug absorption, disposition, elimination using pharmacokinetics, important pharmacokinetic parameters in defining drug disposition and in therapeutics. Mention of uses of pharmacokinetics in drug development process.
- (b) Pharmacodynamics. Introduction, elementary treatment of enzyme stimulation, enzyme inhibition, sulphonamides, membrane active drugs, drug metabolism, xenobiotics, biotransformation, significance of drug metabolism in medicinal chemistry.

(12Hrs)

- 1. Physical Organic Chemistry, Jack Hine, McGraw-Hill.
- 2. Mechanism-An introduction to the study of organic reactions, R.A. Jackson, Oxford Chemistry, Series.
- 3. Medicinal Chemistry, P. Paramoo, CBS, India.
- 4. Introduction to medicinal chemistry, A.Griguage, Wiley-VCH.
- 5. Chemical Kinetics, K.J. Laidler, Tata McGraw-Hill, New Delhi.
- 6. Chemical Kinetics, E.S. Espenson, Tata McGraw-Hill, New Delhi.

## M.Sc. SEMESTER III Course 04 (CHE 301B) (ELECTIVE PAPER IV): Analytical Chemistry

Maximum Marks: 100 (End Sem.:60+CE: 40) Credit: 3

Teaching Hour: 54

#### **UNIT I**

Statistical Analysis. Emphasis should be placed on numerical problems. Significant figures. Accuracy and precision. Errors, systematic and random errors. Propagation of errors. Standard deviation. Coefficient of variation. Confidence limit. Significance test. t-Test, F-Test. Rejection of a result. The least-squares method for deriving calibration graph. Correlation coefficient. Limit of detection.

Sample Preparation for Chromatography. Solid-phase extraction, solid-phase microextraction. Extraction with molecular imprinted polymers.

(10Hrs)

## **UNIT II**

Chromatography. Theory of Chromatography. Retention time. Capacity factor. Number of theoretical plates, and plate height. Band broadening, van Deemter equation. Column resolution.

Gas Chromatography. Instrumentation. Columns. Detection: flame ionisation detector, thermal conductivity detector and mass spectrometric detector.

*High-Performance Liquid Chromatography.* Instrumentation. Pumping systems. Sample injection system. Columns. Detection: UV-Vis detector, photodiode array detector, fluorescence detector, refractive index detector and mass spectrometric detection.

Capillary Electrophoresis. Principle, modes of operation, and instrumentation.

(12Hrs)

## **UNIT III**

*Ion Exchange.* Cation and anion exchangers. Action of ion exchange resins. Ion exchange equilibria and ion exchange capacity. Strongly and weakly acidic cation exchangers. Strongly and weakly basic anion exchangers. Liquid ion exchangers. Ion chromatography. Conductivity detection using suppressor column.

Solvent Extraction. The distribution coefficient. Factors favouring solvent extraction. Extraction reagents. Synergetic effects. Ion-pair extraction. Extraction and stripping. Solvent extraction with crown ethers, and factors influencing it.

(10Hrs)

## UNIT IV

Atomic Absorption Spectrometry. Principle. Instrumentation. Flame atomization. Hollow-cathode lamps. Inductively coupled plasma-mass spectrometry.

*Electrolytic Methods.* Fundamentals of the techniques: Voltammetry. Polarography. Differential pulse polarography. Cyclic voltammetry. Anodic stripping analysis.

(10Hrs)

#### **UNIT V**

Acid-Base Titrations. Kjeldahl method for determination of nitrogen. Determination involving acetylation (amino and hydroxyl groups); and oximation (carbonyl group).

Precipitation Titrations. Argentometric titrations. Mohr titration. Volhard titration. Fajan titration.

Complexometric Titrations. Titration with EDTA. Indicators for EDTA titrations. Titration methods: direct and back titrations, and displacement methods. Masking and demasking agents, and their use in EDTA titrations.

Redox Titrations. Determination of 1,2-diols by periodate oxidation. Karl Fischer titration of water. Determination of DO, BOD and COD.

(12Hrs)

- 1. D.A. Skoog, D.M. West, F.J. Holler and S.R. Crouch, Fundamentals of analytical chemistry, Thomson Brooks/Cole, Singapore.
- 2. D.C. Harris, Quantitative chemical analysis, W.H. Freeman and Co., New York.
- 3. J.D. Christian, Analytical Chemistry, Wiley, New York.
- 4. Principles and Practice of Analytical Chemistry, F.W. Fifield and D. Kealey, Blackwell Publishing.
- 5. S.M. Khopkar, Basic concepts of analytical chemistry, Wiley Eastern, New Delhi.
- 6. S.M. Khopkar, Analytical chemistry of macrocyclic and supramolecular compounds, Narosa Publishing House, New Delhi.
- 7. Vogel's Textbook of Quantitative Analysis, revised, J. Bassett, R. C. Denney, G. H. Jeffery and J. Mendham, ELBS.

## M.Sc. SEMESTER III Course 04 (CHE-301C) (ELECTIVE PAPER IV): Photochemistry

Maximum Marks: 100 (End Sem.:60+CE: 40)

Credit: 3

Teaching Hour: 54

#### Unit-I

Photochemical Reactions. Interaction of electromagnetic radiation with matter, types of excitations, fate of excited molecule, quantum yield, transfer of excitation energy, actinometry.

(10Hrs)

#### Unit II

Determination of Reaction Mechanism. Classification, rate constants and life times of reactive energy state determination of rate constants of reactions. Effect of light intensity on the rate of photochemical reactions. Types of photochemical reactions-photo dissociation, gas-phase photolysis.

(11Hrs)

#### Unit III

Photochemistry of Alkene. Intramolecular reactions of the olefinic bond-geometrical isomerism, cyclisation reactions, rearrangement of 1,4- and 1,5-dienes.

Photochemistry of Aromatic Compounds. Isomerisations, additions and substitutions.

(11Hrs)

## **Unit IV**

Photochemistry of Carbonyl Compounds. Intramolecular reactions of carbonyl compounds-saturated, cyclic and acyclic, unsaturated and  $\alpha,\beta$ -unsaturated compounds, cyclohexadienones. Intermolecular cyloaddition reactions-dimerisations and oxetane formation.

(11Hrs)

## Unit V

*Miscellaneous Photochemical Reactions.* Photo-Fries reactions of annelid's, Photo-Fries rearrangement. Barton reaction. Singlet molecular Oxygen reaction. Photochemical formation of smog. Photodegration of polymers. Photochemistry of vision.

(11Hrs)

- 1. Fundamentals of photochemistry, K.K. Rothagi-Mukheriji, Wiley-Eastern.
- 2. Essentials of Molecular Photochemistry, A Gilbert and J. Baggott, Blackwell Scientific Publication.
- 3. Molecular Photochemistry, N.J. Turro, W.A. Benjamin.
- 4. Introductory Photochemistry, A. Cox and t. Camp, McGraw Hill.
- 5. Photochemistry, R.P. Kundall and A. Gilbert. Thomson Nelson.
- 6. Organic Photochemistry, J. Coxon and B.halton, Cambridge University Press.
- 7. Photochemistry and pericyclic reactions, J. Singh and J. Singh, New Age International, New Delhi.
- 8. Photochemistry, R. P. Kundall and A. Gilbert, Thomson Nelson.

## M.Sc. SEMESTER III Course 04 (CHE-301D) (ELECTIVE PAPER IV): Biochemistry

Maximum Marks: 100 (End Sem.:60+CE: 40) Credit: 3

**Teaching Hour: 54** 

#### Unit I

Metal Ions in Biological Systems. Bulk and trace metals with special reference to Na, K, Mg, Ca, Fe, Cu, Zn, Co, and K+/Na+ pump.

Bioenergetics and ATP Cycle. DNA polymerisation, glucose storage, metal complexes in transmission of energy; chlorophyll's, photosystem I and photosystem II in cleavage of water.

Transport and Storage of Dioxygen. Heam proteins and oxygen uptake structure and function of haemoglobin's, mygolobin, haemocyanms and hemerythrin, model synthetic complexes of iron, cobalt and copper.

(10Hrs)

#### Unit II

*Electron Transfer in Biology.* Structure and function of metal of proteins in electron transport processes cytochrome's and ion-sulphure proteins, synthetic models.

Nitrogen fixation. Biological nitrogen fixation, and its mechanism, nitrogenase, Chemical nitrogen fixation.

(10Hrs)

## **Unit III**

*Enzymes*. Introduction and historical perspective, chemical and biological catalysis, remarkable properties of enzymes like catalytic power, specificity and regulation. Nomenclature and classification, extraction and purification. Fischer's lock and key and Koshalnd's induced fit hypothesis, concept and identification of active site by the use of inhibitors, affinity labeling and enzyme modification by site-directed mutagenesis. Enzyme kinetics, Michael's-Menten and Lineweaver Burk plots, reversible and irreversible inhibition.

Mechanism of Enzyme Action. Transition-state theory, orientation and Steric effect, acid-base catalysis, covalent catalysis, strain or distortion. Examples of some typical enzyme mechanisms for chemotrypsin, ribonuclease, lysozyme and carboxypeptidase.

Kinds of Reactions Catalysed by Enzymes. Nucleophilic displacement on a phosphorus atom, multiple displacement reactions and the coupling of ATP cleavage to endergonic processes. Transfer of sulphate, addition and elimination reactions, enolic intermediates in Isomerisations reactions, b-Cleavage and condensation, some isomerization and rearrangement reactions. Enzyme catalyzed carboxylation and decarboxylation.

(12Hrs)

## **Unit IV**

Co-Enzyme Chemistry. Cofactors as derived from vitamines, coenzymes, prosthetic groups, apoenzymes. Structure and biological functions of coenzyme A, thiamine pyrophosphate, pyridoxal phosphate, NAD+, NADP+, FMN, FAD, lipoic acid, vitamin B12. Mechanisms of reactions catalyzed by the above cofactors. Enzyme Models. Host-guest chemistry, chiral recognition and catalysis, molecular recognition, molecular asymmetry and prochirality Biometric chemistry, crown ether, cryptates. Cyclodextrins, cyclodextrion-based enzyme models, clixarenes, ionospheres, micelles synthetic enzymes or synzymes.

Biotechnological Applications of Enzymes. Large-scale prodcution and purification of enzymes, techniques and methods of immobilization of enzymes, effect of immobilization on enzyme activity, application of immobilized enzymes, use of enzymes in food and drink industry-brewing and cheesemaking, syrups from cron starch, enzymes as targets for drug design. Clinical uses of enzymes, enzyme therapy, enzymes and recombinant DNA Technology.

(11Hrs)

#### Unit V

Biological Cell and its Constituents. Biological cell, structure and functions of proteins, enzymes, DNA and RNA in living systems. Helix coils transition.

*Bioenergetics.* Standard free energy change in biochemical reactions, exergonic, endergonic. Hydrolysis of ATP, synthesis of ATP from ADP.

Biopolymer Interactions. Forces involved in biopolymer interactions. Electrostatic charges and molecular expansion, hydrophobic forces, dispersion force interactions. Multiple equilibrium and various types of bidning processes in biological systems. Hydrogen ion titration curves.

Cell Membrane and Transport of Ions. Structure and functions of cell membrane, ion transport through cell membrane, irreversible thermodynamic treatment of membrane transport. Nerve conduction.

(11Hrs)

- 1. Biochemistry, D. Voet and J.G. Voet, John Wiley.
- 2. Principles of Biochemistry, A.L. Lehninger, D.L. Nelson and M.M. Cox, CBS Publishers, Delhi.
- 3. Principles of Bioinorganic Chemistry, S.J. Lippard and J.M. Berg, University Science Books.
- 4. Bioinorganic Chemistry, 1. Bertini, H.B. Gray, S.J. Lippard and J.S. Valentine, University Science Books.

- Inorganic biochemistry vol. I and II ed. G.L. Eichhorn, Elsever.
- 6. Progress in Inorganic Chemistry, Vol 18 and 38 ed J.J. Lippard, Wiley.
- 7. Bioorganic Chemistry: A chemical Approach to Enzyme Action, Hermann Dugas and C. Penny, Springer Verlag.
- 8. Understanding Enzymes, Trevor Palmer, Prentice Hall.
- Enzyme Chemistry: Impact and applications, Ed. Collin J suckling, chemistry.
- 10. Enzyme Mechanisms Ed. M.I. Page and A Williams, Royal Society of Chemistry.
- 11. Fundamentals of Enzymology, N.C. Price and L. Stevens. Oxford University Press.
- 12. Immobilized Enzymes: An Introduction and Applications in Biotechnology, Michael ID. Trevan, Hohn Wiley.
- 13. Enzymatic Reaction Mechanisms. C. Walsh. W.H. Freeman.
- 14. Enzyme Structure and Mechanism, A Fersht, W.H. Freeman
- 15. Biochemistry: The Chemical Reactions of Living Cells, D.E. Metzler, Academic Press.

## M.Sc. SEMESTER III Course 05 (CHE-302A) (ELECTIVE PAPER V): Theoretical Chemistry

Maximum Marks: 100 (End Sem.:60+CE: 40) Credit: 3 Teaching Hour: 54

## **UNIT I**

Quantum Mechanics. Review of the principles of quantum mechanics, Born-Oppenheimer approximation and its breakdown, Slater rules, Hartree-Fock equation.

(10Hrs)

## **UNIT II**

Statistical Thermodynamics: Part I. Postulates of statistical mechanics, Maxwell-Boltzmann distribution law of molecular velocities and energies. Distinguishability of particles-quantum statistics, Bose-Einstein and Fermi-Dirac statistics; comparison of Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac statistics. Application of Fermi-Dirac and Bose-Einstein statistics.

(11Hrs)

## **UNIT III**

- (a) Statistical Thermodynamics: Part II. Entropy and probability, partition functions, translational, vibrational and rotational partition functions, Sackur-Tetrode equation. Relation of partition function with entropy, free energy and weak function. Application of partition function.
  - (b) Specific heat of solids-Einstein and Debye models, their weaknesses.

(11Hrs)

#### **UNIT IV**

*Irreversible Thermodynamics.* Thermodynamic criteria for non-equilibrium states, entropy productin and entropy flow, transformation of the generalised fluxes and forces, non-equilibrium stationary states, phenomenological equations, microscopic reversibility and Onsager's reciprocity relations, electrokinetic phenomena, diffusion, electric conduction, coupled reactions.

(11Hrs)

## **UNIT V**

*Enzymes.* Introduction and historical perspective, chemical and biological catalysis, remarkable properties of enzymes such as catalytic power, specificity and regulation. Nomenclature and classification, extraction and purification. Fischer's lock and key and Koshland's induced fit hypothesis, concept and identification of active site by the use of inhibitors, affinity labeling and enzyme modification by site-directed mutagenesis. Enzyme kinetics, Michaelis-Menten and Lineweaver-Burk plots, reversible and irreversible inhibition.

(11Hrs)

- 1. Theoretical Chemistry, S. Glasstone, East-West, India.
- 2. Quantum Chemistry, Eyring and Kimball.
- 3. Introduction to Thermodynamics of Irreversible Processes, I. Prigogine, C.C. Thomas Publishers.
- 4. Irreversible Thermodynamics, R.C. Shrivastava, Prentice-Hall, India.
- 5. Principles of Enzyme Kinetics. Athel Cornish-Bowden.
- 6. Physical Chemistry, P.W. Atkins, ELBS.

## M.Sc. SEMESTER III Course 05 (CHE-302B) (ELECTIVE PAPER V): Chemistry of Materials

Maximum Marks: 100 (End Sem.:60+CE: 40) Credit: 3

Teaching Hour: 54

#### **UNIT I**

Ceramics, Composites and Nanomaterials. Ceramic structures, mechanical properties, clay products. Refractories, characterization, properties and applications. Microscopic composites, dispersion-strengthened and particle-reinforced composites, macroscopic composites. Nanocrystalline phase, preparation procedures, properties and applications.

(11Hrs)

#### **UNIT II**

Liquid Crystals. Thermotropic liquid crystals, positional order, bond orientational order, nematic and smectic mesophases. Molecular arrangement in smectic A and smectic C phases, optical properties of liquid crystals. Dielectric susceptibility and dielectric constants. Lyotropic phases and their description of ordering in liquid crystals.

(11Hrs)

### **UNIT III**

*Ionic Conductors*. Types of ionic conductors, mechanism of ionic conduction, interstitial jumps (Frenkel); vacancy mechanism, diffusion superionic conductors, phase transtions and mechanism of conduction in superionic conductors. Examples and applications of ionic conductors.

(10Hrs)

#### **UNIT IV**

High Tc Materials. High Tc superconductivity. Preparation and characterization of 1-2-3 and 2-1-4 materials. Normal state properties, anisotropy, temperature dependence of electrical resistance, and optical phonon modes. Superconducting state; heat capacity; coherence length, elastic constants, microwave absorption-pairing and multigap structure in high Tc materials. Applications of high Tc materials.

(11Hrs)

## **UNIT V**

Organic Solids, Fullerenes, Molecular Devices. Conducting organics, organic superconductors, magnetism in organic materials. Fullerenes, doped, fullerenes as superconductors. Molecular rectifiers and transistors, artificial photosynthetic devices, optical storage memory and switches, sensors.

Non-linear optical materials, non-linear optical effects, Molecular hyperpolarisability,

(11Hrs)

- 1. Material Science and Engineering-An Introduction, W.D. Callister, Wiley.
- Solid State Physics, N.W. Ashcroft and N.D. Mermin, Saunders College.
- 3. Principles of the Solid State, H.V. Keer, Wiley Eastern.
- 4. Materials Science, J.C. Anderson, K.D. Leaver, J.M. Alexander and R.D. Rawlings, ELBS.
- 5. Thermotropic Liquid Crystals, G.W. Gray, editor, John Wiley.
- 6. Handbook of Liquid Crystals, Kelker and Hatz, Chemie Verlag.

## M.Sc. SEMESTER III Course 05 (CHC-302EC) (ELECTIVE PAPER V): Electrochemistry

Maximum Marks: 100 (End Sem.:60+CE: 40)

Credit: 3
Teaching Hour: 54

#### Unit I

Conversion and Storage of Electrochemical Energy Present status of energy consumption. Pollution problem. History of fuel cells, Direct energy conversion by electrochemical means. Maximum intrinsic efficiency of an electrochemical converter. Physical interpretation of the Carnot efficiency factor in electrochemical energy converters. Power outputs. electrochemical Generators (Fuel Cells): Hydrogen oxygen cells, Hydrogen Air cell, Hydrocarbon air cell, Alkane fuel cell, Phosphoric and fuel cell, direct NaOH fuel cells, applications of fuel cells.

Electrochemical Energy Storage. Properties of Electrochemical energy storage: Measure of battery performance, Charging and discharging of a battery, Storage Density, Energy Density. Classical Batteries: (i) Lead Acid (ii) Nickel-Cadmium, (iii) Zinc manganese dioxide. Modern Batteries: (i) Zinc-Air (ii) Nickel-Metal Hydride, (iii) Lithium Battery, Future Electricity storers: Storage in (i) Hydrogen, (ii) Alkali Metals, (iii) Non aqueous solutions.

(12Hrs)

## **Unit II**

Corrosion and Stability of Metals. Civilization and Surface mechanism of the corrosion of the metals; Thermodynamics and the stability of metals, Potential -pH (or Pourbaix) Diaphragmsl; uses and abuses, Corrosion current and corrosion potential -Evans diagrams. Measurement of corrosion rate: (i0 Weight Loss method, (ii) Electrochemical Method.

Inhibiting Corrosion. Cathodic and Anodic Protection. (i) Inhibition by addition of substrates to the electrolyte environment, (ii) by charging the corroding method from external source, anodic Protection, Organic inhibitors, The fuller Story Green inhibitors.

Passivation. Structure of Passivation films, Mechanism of Passivation, Spontaneous Passivation Nature's method for stabilizing surfaces.

(11Hrs)

#### **Unit III**

*Bioelectrochemistry.* bioelectrodics, Membrane Potentials, Simplistic theory, Modern theory, Electrical conductance in biological organism: Electronic, Protonic electrochemical mechanism of nervous systems, enzymes as electrodes.

Kinetic of Electrode Process. Essentials of Electrode reaction. Current Density, Overpotential, Tafel Equation, Butler Volmer equation. Standard rate constant (K0) and Transfer coefficient (a), Exchange Current.

Irreversible Electrode processes. Criteria of irreversibility, informatino from irreversible wave.

(11Hrs)

#### **Unit IV**

Methods of determining kinetic parameters for quasi-rversible and irreversible waves. Koutecky's methods, Meits Israel Method, Gellings method.

*Electrocatalysis.* Chemical catalysts and Electrochemical catalysts with special reference to purostates, porphyrin oxides of rare earths. Electrocatalysis in simple redox reactions, in reaction involving adsorbed species. Influence of various parameters.

(10Hrs)

## Unit V

Potential Sweep Method. Linear sweep Voltammetry, Cyclic Voltammetry, theory and applications. Diagnostic criteria of cycli voltammetry. Controlled current microelectrode techniques: comparison with controlled potentials methods, chronopotentiometry, theory ad applications.

Bulk Electrolysis Methods. Controlled potential coulometry, Controlled Coulometry, Electroorganic synthesis and its important applications. Stripping analysis: anodic and Cathodic modes, Pre electrolysis and Stripping steps, applications of Stripping Analysis.

(10Hrs)

- 1. Modern Electrochemistry Vol. I, IIa, Vol. IIB J'OM Bockris and A.K.N. Reddy, Plenum Publication, New York.
- 2. Polarographic Techniques by L. Meites, Interscience.
- 3. "Fuel Cells: Thjeir electrochemistry". McGraw Hill Book Company, New York.
- 4. Modern Polarographic Methods by A.M. Bond, Marcell Dekker.
- 5. Polarography and allied techniques by K. Zutshi, New age International Publicatin. New Delhi.
- 6. "Electroaalytical Chemistry by Basil H. Vessor & Galen W.; Wiley Interscience.
- 7. Electroanalytical Chemistry by Basil H. Vessor & alen w.; Wiley Interscience.
- 8. Topics in pure and Applied Chemistry, Ed. S. K. Rangrajan, SAEST Publication, Karaikudi (India)

## M.Sc. SEMESTER III Course 05 (CHE-305D) (ELECTIVE PAPER V): Medicinal Chemistry

Maximum Marks: 100 (End Sem.:60+CE: 40) Credit: 3 Teaching Hour: 54

#### Unit I

Structure and activity. Relationship between chemical structure and biological activity (SAR). Receptor Site Theory. Approaches to drug design. Introduction to combinatorial synthesis in drug discovery. Factors affecting bioactivity. QSAR-Free-Wilson analysis, Hansch analysis, relationship between Free-Wilson analysis and Hansch analysis.

(12Hrs)

## Unit II

*Pharmacodynamics.* Introduction, elementary treatment of enzymes stimulation, enzyme inhibition, sulfonamides, membrane active drugs, drug metabolism, xenobiotics, biotransformation, significance of drug metabolism in medicinal chemistry.

(11Hrs)

#### Unit III

Antibiotics and antibacterials. Introduction, Antibiotic  $\beta$ -Lactam type - Penicillins, Cephalosporins, Antitubercular. Streptomycin, Broad spectrum antibiotics . Tetracyclines, Anticancer – Dactinomycin (Actinomycin D)

(11Hrs)

## **Unit IV**

Antifungal polyenes, Antibacterials. Ciprofloxacin, Norfloxacin, Antiviral. Acyclovir Antimalarials. Chemotherapy of malaria. SAR. Chloroquine, Chloroquanide and Mefloquine

(10Hrs)

#### Unit V

Non-steroidal Anti-inflammatory Drugs. Diclofenac Sodium, Ibuprofen and Netopam Antihistaminic and antiasthmatic agents: Terfenadine, Cinnarizine, Salbutamol and Beclomethasone dipropionate.

(10Hrs)

- Introduction to Medicinal Chemistry, A Gringuage, Wliey-VCH.
- 2. Wilson and Gisvold's Text Book of Organic Medicinal and Pharmaceutical Chemistry, Ed. R.F. Dorge.
- 3. An Introduction to Drug Design, S.S. Pandeya and J.R. Dimmock, New Age International.
- 4. The Organic Chemistry of Drug Design and Drug Action, R.B. Silverman, Academic Press.
- 5. Strategies for Organic Drug Synthesis and design, D. Lednicer, John wiley.

# PRACTICAL COURSES M.Sc. SEMESTER III Project report COURSES 06 (CHC-306)

Maximum Marks: 100

Credit: 9 Teaching Hour: 90

The submit project report may be undertaken in any of the National laboratories /institute /universities/ government approved companies / industries

| Course 06 | Project report | Max. Marks 50 | Credit: | 9 |
|-----------|----------------|---------------|---------|---|
| CHC 304:  | Presentation   | Max. Marks 50 |         |   |

## M.Sc. SEMESTER IV Course 01 (CHC-401) (PAPER I): Inorganic Chemistry

Maximum Marks: 100 (End Sem.:60+CE: 40)

Credit: 3 Teaching Hour: 54

## **UNIT I**

*Electron Spin Resonance Spectroscopy.* Basic principles, hyperfine and superhyperfine splitting, g value and factors affecting g values, applications to transition metal complexes.

(12Hrs)

#### UNIT I

Mössbauer Spectroscopy. Basic principles, spectral parameters and spectrum display. Application of the technique to the studies of (1) bonding and structures of  $Fe^{+2}$  and  $Fe^{+3}$  compounds including those of intermediate spin, (2)  $Sn^{+2}$  and  $Sn^{+4}$  compounds -nature of M-L bond, coordination number, structure and (3) detection of oxidation state.

(12Hrs)

### **UNIT-III**

Application of group theory to Spectroscopy. Use of group theory in predicting IR and Raman active modes in some simple molecules of  $C_{2v}$ ,  $C_{3v}$  and  $D_{\infty h}$  point groups.

(10Hrs)

## **UNIT IV**

*Bioinorganic Chemistry.* Metal complexes in transmission of energy; chlorophylls, photosystem-I and photosystem-II in cleavage of water, model systems.

(10Hrs)

#### Unit V

Electron Transfer in Biology: Structure and function of metalloproteins in electron transport processes-cytochromes and ion-sulphur proteins. Nitrogenase: Biological nitrogen fixation, molybdenum nitrogenase-structure and function.

10Hrs)

- Principles of Bioinorganic Chemistry, S.J. Lippard and J.M. Berg, University Science Books.
- 2. Bioinorganic Chemistry, I. Bertini, H.B. Gray, S.J. Lippard and J.S. Valentine, University Science Books.
- 3. Inorganic Biochemistry vols I and II. ed. G.L. Eichturn, Elsevier.
- 4. Progress in Inorganic Chemistry, Vols 18 and 38 ed. J.J. Lippard, Wiley, Environmental Chemistry, S. E. Manahan, Lewis Publishers.

## M.Sc. SEMESTER IV Course 02 (CHC-402) (PAPER II): Organic Chemistry

Maximum Marks: 100 (End Sem.:60+CE: 40)

Credit: 3 Teaching Hour: 54

### **UNIT I**

<sup>13</sup>C-NMR Spectroscopy General considerations, chemical shift (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbon), wide band H-decoupled and off-resonance H-decoupled spectra. Calculation of chemical shift values for alkanes and substituted benzene.

Two dimension NMR spectroscopy. COSY, and DEPT techniques.

Conjoint Spectroscopy Problems. Application of UV, IR, Raman, NMR and Mass spectrometry for elucidation of structure of organic compounds. (10Hrs)

#### **UNIT II**

Mass Spectrometry-Part I. Ion production, electron ionisation (EI), chemical ionisation (CI), field desorption (FD), field ionisation (FI), and fast atom bombardment (FAB). Atmospheric pressure ionisation techniques. Electrospray ionisation, and atmospheric pressure chemical ionisation. Thermospray ionisation. Matrix assisted laser desorption ionisation (MALDI).

Mass analysers. Magnetic sector analysers. Quadrupolar analysers, ion trap, time-of-flight (TOF), ion cyclotron resonance (ICR). Electron multiplier. Tandem mass spectrometry (MS/MS).

(11Hrs)

## **UNIT III**

Mass Spectrometry-Part II. Isotopic abundance. Electron ionisation and fragmentation (positive ions). Molecular ion peak, metastable peak. McLafferty rearrangement. Nitrogen rule. Parity rule. Mass spectral fragmentation of organic compounds containing common functional groups (alkanes, alkenes, alkynes, halo-compounds, alcohols, amines, carbonyl compounds, aromatic compounds).

High resolution mass spectrometery. Interpretation of mass spectra. Problems based on mass spectrometry of organic compounds.

(11Hrs)

## **UNIT IV**

Elimination Reactions. The E2, E1 and E1cB mechanisms and their spectrum. Orientation of the double bond. Reactivity, effect of substrate structure, attacking base, the leaving group and the medium. Elimination *versus* substitution. Mechanism and orientation in pyrolytic elimination. The Hofmann degradation. Dihalo-elimination. Decomposition of toluene-p-sulphonylhydrazones. Conversion of ketoximes to nitriles. *N*-Nitrosoamine to diazoalkane transformation.

(10Hrs)

## **UNIT V**

*Enzymes.* Properties of enzymes, catalytic power, specificity and regulation. Fischer's lock and key and Koshland's induced fit hypothesis. Identification of active site by the use of inhibitors.

*Kinetics.* Transition-state theory. Michaelis-Menten equation, and Lineweaver-Burk plot. Enzyme mechanisms for chymotrypsin, lysozyme and carboxypeptidase A.

Coenzyme chemistry. Structure and biological functions of coenzyme A, thiamine pyrophosphate, pyridoxal phosphate, NAD<sup>+</sup>, NADP<sup>+</sup>, FMN, FAD, and vitamin B<sub>12</sub>.

Methods of immobilization of enzymes. Effect of enzyme immobilization on enzyme activity.

(12Hrs)

- 1. Introduction to Spectroscopy, D.L. Pavia, G.M. Lampman and G.S. Kriz, Thomson, Brooks/Cole.
- 2. Organic Spectroscopy, W. Kemp, ELBS, Macmillan.
- 3. Spectrometric Identification of Organic Compounds, R. M. Silverstein, G.C. Bassler and T.C, Morrill, John Wiley
- Spectroscopic Methods in Organic Chemistry, D. H. Williams, I. Fleming, Tata McGraw-Hili.
- 5. Application of Spectroscopy of Organic Compounds, J. R. Dyer, Prentice Hall.
- 6. Mass Spectrometry, E. de Hoffmann and V. Stroobant, Wiley, Chichester.
- 7. Ionization Methods in Organic Mass Spectrometry, A.E. Ashcroft, Royal Society of Chemistry, Cambridge.
- 8. Organic Chemistry, J. Claden, N. Greeves, S. Warren, P. Wothers, Oxford University Press.
- 9. Organic Chemistry, L.G. Wade, Jr., Pearson Education
- 10. Advanced Organic Chemistry-Reactions, Mechanism and Structure, Jerry March, Wiley-Interscience.
- 11. Biochemistry, D. Voet and J.G. Voet, John Wiley.
- 12. Principles of Biochemistry, A.L. Lehninger, D.L. Nelson and M.M. Cox, CBS Publishers, Delhi.
- 13. Immobilized Enzymes: An Introduction and Applications in Biotechnology, Michael D. Trevan, John Wiley.

## M.Sc. SEMESTER IV Course 03 (CHC-403) (PAPER III): Physical Chemistry

Maximum Marks: 100 (End Sem.:60+CE: 40)

Credit: 3 Teaching Hour: 54

#### **UNIT I**

*Nuclear Magentic Resonance Spectroscopy.* Nuclear spin, nuclear resonance, saturation, shielding of magnetic nuclei, chemical shift and its measurement, factors influencing chemical shift, deshielding, spin-spin interactions, factors influencing coupling constant, J. Exchange phenomenon.

(12Hrs)

## **UNIT II**

*Electron Spin Resonance Spectroscopy.* Basic principles, zero field splitting and Kramer's degeneracy, factors affecting the g value. Hyperfine coupling. Double resonance in esr. Spin Hamiltonian relationship, measurement techniques, applications.

(12Hrs)

#### **UNIT III**

Photochemistry. Thermal and photochemical reactions. Laws of photochemistry, quantum yield and its determination, abnormal quantum yield, primary and secondary processes; Fluorescence and phosphorescence, chemiluminescence, photosensitation. Photogalvanic and photocatalytic effects.

(10Hrs)

#### **UNIT IV**

Steric and Conformational Properties. Various types of steric strain and their influence on reactivity. Steric acceleration. Primary and secondary steric effects, LFER. Conformational barrier to bond rotation-spectroscopic detection of individual conformers. Winstein-Holness and Curtin-Hammett principle.

(10Hrs)

#### **UNIT V**

Nucleophilic and Electrophilic Reactivity. Structural and electronic effects on  $S_N1$  and  $S_N2$  reactivity. Solvent effects on nucleophilic displacements. Kinetic isotope effects. Intramolecular assistance. Electronic effects and reactivity in  $S_N2$  reaction, curve-crossing model. Relationship between polar and electron transfer reactions.

(10Hrs)

- 1. Quantum Chemistry, Eyring and Kimball.
- 2. Quantum Mechanics, Hanna.
- 3. Introduction to Quantum Chemistry, A.K. Chandra.
- Physical Chemistry, P.C. Rakshit.
- 5. Physical Chemistry, P.W. Atkins, ELBS.
- 6. Solid State Chemistry, N.B. Hannay, Prentice-Hall, India
- 7. Fundamentals of Molecular Spectroscopy, C.N. Banwell, Tata McGraw-Hill, New Delhi.
- 8. Basic Physical Chemistry, W.J. Moore, Prentice-Hall, India.
- 9. Physical Methods in Chemistry, R.S. Drago.
- 10. Applied Electron spectroscopy for Chemical Analysis, H. Windawi and F.L. Ho, editors, Wiley Interscience.
- 11. Introduction to Molecular Spectroscopy, G.M. Barrow, McGraw-Hill.
- 12. Basic Principles of Spectroscopy, R. Chang, McGraw-Hill.
- 13. Physical Organic Chemistry, Jack Hine, McGraw-Hill.
- 14. Mechanism-An Introduction to the Study of Organic Reactions, R.A. Jackson, Oxford Chemistry Series.
- 15. Structure and Mechanism in Organic Chemistry, C.K. Ingold, G. Bell & Sons.
- 16. Physical Organic Chemistry, N.S. Issacs, ELBS, Longman.

## M.Sc. SEMESTER IV Course 04 (CHE-401A) (ELECTIVE PAPER IV): Organic Synthesis

Maximum Marks: 100 (End Sem.:60+CE: 40) Credit: 3

**Teaching Hour: 54** 

#### **UNIT I**

Designing organic synthesis. The Disconnection Approach. Basic principles, synthons, functional group interconversions. Order of events in organic synthesis. One group C-X disconnections and two group C-X disconnections. Chemoselectivity. Reversal of polarity (umpolung). Amine synthesis.

(10Hrs)

## **UNIT II**

Organoboranes. Preparation of organoboranes and their synthetic applications. Oxidation, protonolysis and isomerisation. Carbonylation of organoboranes. Cyanoborate process. Reaction of alkenyl boranes and trialkylalkynyl borates.

*Organosilanes.* Synthetic applications of trimethylsilyl chloride, trimethylsilyl cyanide, trimethylsilyl iodide and trimethylsilyl triflate.

Synthetic applications of  $\alpha$ -silyl carbanions and  $\beta$ -silyl carbonium ions.

(11Hrs)

## **UNIT III**

*Oxidation.* Oxidation of carbon-carbon double bond. Perhydroxylation, potassium permanganate, osmium tetroxide, iodine together with silver carboxylates, ozonolysis. Enantioselective epoxidation of allylic alcohols (Sharpless epoxidation).

Oxidation of alcohols. Chromic acid, chromiun (VI) oxide-pyridine complexes, manganese (IV) oxide, silver carbonate, oxidation via alkoxysulphonium salts.

Baeyer-Villiger oxidation of ketones.

Oxidation with ruthenium tetroxide, thallium(III) nitrate and iodobenzene diacetate.

(12Hrs)

#### **UNIT IV**

Reduction. Catalytic hydrogenation (homogeneous and heterogenous). Stereochemicstry and mechanism, selectivity of reduction.

Reduction by dissolving metals. Metal and acid, metal and alcohol, metal and ammonia.

Reduction by hydride-transfer reagents. Aluminium alkoxides, lithium aluminium hydride, sodium borohydride, lithium hydrido-alkoxyaluminates.

Wokff-Kishner reduction. Reduction with di-imide.

(11Hrs)

## **UNIT V**

Phase transfer catalysis, principle and applications.

Basic principles of convergent and linear synthesis.

Stereospecific and stereoselective synthesis. Regioselectivity.

Synthetic uses of lead tetraacetate, N-bromosuccinimide, selenium dioxide, dialkyl lithium cuprate, lithium diisopropylamide. Umpolung reaction.

(10Hrs)

- S. Warren, Organic synthesis: The disconnection approach, John Wiley, Chichester.
- 2. W. Carruthers, Modern methods of organic synthesis, Cambridge University Press, Cambridge.
- 3. R.E. Ireland, Organic synthesis, Prentice-Hall of India, New Delhi.
- 4. R. Bruckner, Advanced organic chemistry: Reaction and mechanism, Harcourt (India), New Delhi.
- 5. H.O. House and W.A. Benjamin, Modern synthetic reactions.
- 6. F.A. Carey and R.J. Sundgerg, Advanced organic chemistry, Plenum.
- 7. J. March, Advanced organic chemistry: Recations, mechanism, structure, Wiley.

## M.Sc. SEMESTER IV Course 04 (CHE-401B) (ELECTIVE PAPER IV): Polymers

Maximum Marks: 100 (End Sem.:60+CE: 40) Credit: 3

Teaching Hour: 54

#### **UNIT I**

Basics of Polymers. Repeating units, degree of polymerisation, linear, branched and network polymers. Classification of polymers. Addition, radical, ionic, coordination and condensation polymerisation; their mechanism and examples.

Polymerisation conditions and polymer reactions. Polymerisation in homogeneous and heterogeneous systems.

(10Hrs)

#### **UNIT II**

Polymer Characterisation. Significance of molecular weight of polymer. Polydispersive average molecular weight. Number, weight and viscosity average weights. Measurement of molecular weights. End group, viscosity, light scattering, osmotic and ultracentrifugation methods.

Chemical and spectroscopic analysis of polymers. X-Ray diffraction study. Thermal analysis, tensile strength, fatique, impact. Tear resistance. Hardness and abrasion resistance.

(12Hrs)

## **UNIT III**

Structure and Properties. Configuration of polymer chains. Crystal structure of polymers. Morphology of crystalline polymers. Polymer structure and physical properties; crystalline melting point Tm, melting points of homogeneous series, effect of chain flexibility and other steric factors, entropy and heat of fusion. The glass transition temperature, Tg relationship between Tm and Tg, effects of molecular weight, diluents, chemical structure, chain topology, branching and cross linking. Property requirements and polymer utilization.

(12Hrs)

## **UNIT IV**

*Polymer Processing.* Plastics, elastomers and fibres. Compounding. Processing techniques, Calendering, die casting, rotational casting, film casting, injection moulding, blow moulding, extrusion moulding, thermoforming, foaming, reinforcing and fibre spinning.

(10Hrs)

## UNIT V

*Properties of Polymers.* Properties of polyethylene, polyvinyl chloride, polyamides, polyesters, phenolic resins, epoxy resins and silicone polymers.

Functional polymers. Fire retarding polymers, and electrically conducting polymers.

Biomedical polymers, contact lens, dental polymers, artificial heart, kidney, skin and blood cells.

(10Hrs)

- Textbook of Polymer Science, F.W. Billmeyer, Jr., Wiley.
- Polymer Science, V.R. Gwariker, N.V. Viswanathan and J. Sreedhar, Wiley-Eastern.
- 3. Functional Monomers and Polymers, K. Takemoto, Y. Inaki and R.M. Ottanbrite.
- 4. Contomporary Polymer Chemistry, H.R. Alcock and F.W. Lambe, Prentice Hall.
- Physics and Chemistry of Polymers, J.M.G. Cowie, Blackie Academic and Professional.

## M.Sc. SEMESTER IV Course 04 (CHE-401C) (ELECTIVE PAPER IV): Organo Transitional Metal Chemistry

Maximum Marks: 100 (End Sem.:60+CE: 40) Credit: 3

**Teaching Hour: 54** 

#### **UNIT I**

Alkyls, Aryls and hydrides of Transition Metals. Types, routes of synthesis, stability and decomposition pathways and bonding schemes of transition metal alkyls and aryls. Transition metal compounds with bonds to hydrogen: Synthetic methods, characterization and chemical behaviour of transition metal hydrido compounds.

(12Hrs)

## **UNIT II**

Compounds of Transition Metal-Carbon Multiple Bonds. Alkylidenes, alkylidynes, low-valent carbenes and carbynes-synthesis, Nature of bond, structural characteristics, nucleophilic and electrophilic reactions on ligands, role in organic synthesis.

(11Hrs)

#### **UNIT III**

Transition Metal  $\pi$ -Complexes. Transition metal complexes with unsaturated organic molecules like alkenes, alkynes, allyl, diene, dienyl and arene complexes: preparations, properties, nature of bonding and structural features.

(11Hrs)

#### **UNIT IV**

Homogeneous Catalysis. Stoichiometric reactions for catalysis and homogeneous catalytic hydrogenation, Zeigler-Natta polymerization of olefin, catalytic reactions involving hydrocabonylation of olefins (oxo reaction), activation of C-H bonds.

(10Hrs)

## **UNIT V**

Fluxional Organometallic Compounds. Fluxionality and dynamic equilibria in compounds such as  $\eta^2$ -olefin,  $\eta$ 3-allyl and dienyl complexes.

(10Hrs)

- Principles and Applications of Organotransition metal Chemistry, J. P. Collaman, L. S. Hegsdus, J. R. Norton and R. G. Finke, University Science Books.
- 2. The Organometallic Chemistry of the Transition Metals, R. H. Crabtree, John Wiley.
- 3. Organometallic Chemistry, R. C. Mehrotra and A. Singh, New age International.
- 4. Metallo-organic Chemistry, A. J. Pearson, John Wiley.

## M.Sc. SEMESTER IV Course 04 (CHE-401D) (ELECTIVE PAPER IV): Solid State Chemistry

Maximum Marks: 100 (End Sem.:60+CE: 40) Credit: 3

**Teaching Hour: 54** 

#### Unit I

Solid State Reactions. General principles, experimental procedure, co-precipitation as a precursory to solid state reactions, kinetics of solid state reactions.

(10Hrs)

## **Unit II**

Crystal Defects and Non-Stoichiometry. Perfect and imperfect crystals, intrinsic and extrinsic defects-point defects, line and plane defects, vacancies-Schottky detects and Frenkel defects. Thermodynamics of Schottky and Frenkel defect formation, colour centres, non-stoichiometry and defects.

#### Unit III

Electronic Properties and Band Theory. Metal's insulators and semiconductors, electronic structure of solidsband theory band structure of metals, insulators and semiconductors, Intrinsic and extrinsic semiconductors, doping semiconductors, p-n junctions, super conductors. Optical properties-Application of optical and electron microscopy. Magnetic Properties-Classification of materials: Effect of temperature calculation of magnetic moment, mechanism of ferro and anti ferromagnetic ordering super exchange.

(12Hrs)

## **Unit IV**

*Organic Solids.* Electrically conducting solids. organic charge transfer complex, organic metals, new superconductors.

(10Hrs)

## **Unit IV**

*Liquid Crystals.* Types of liquid crystals: Nematic, Smectic, Ferroelectric, Antiferroelectric, Various theories of LC, Liquid crystal display, New materials.

(11Hrs)

- 1. Solid state chemistry and its applications, A.R. West. Peenum.
- 2. Principles of the Solid State, H.V. Keer, Wiley Eastern.
- 3. Solid State Chemistry, N.B. Hannay.
- 4. Solid State Chemistry, D.K. Chakrabarty, New Wiley Eastern.

## M.Sc. SEMESTER IV Course 05 (CHE-402A) (ELECTIVE PAPER V): Chemistry of Natural Products

Maximum Marks: 100 (End Sem.:60+CE: 40) Credit: 3 Teaching Hour: 54

#### **UNIT I**

*Terpenoids.* General methods of structure elucidation. Isoprene rule.

Structure determination, stereochemistry, and synthesis of the following representative molecules: citral, geraniol,  $\alpha$ -terpineol, menthol,  $\alpha$ -pinene, camphor, and abietic acid. Biosynthesis of terpenoids.

(11Hrs)

## **UNIT II**

Alkaloids. General methods of structure elucidation.

Structure determination, stereochemistry, and synthesis of the following representative molecules: ephedrine, nicotine, atropine, quinine and morphine. Biosynthesis of alkaloids.

(10Hrs)

#### **UNIT III**

*Steroids.* Structure elucidation, stereochemistry and chemical synthesis of cholesterol, bile acids, androsterone, testosterone, estrone, progestrone and aldosterone. Biosynthesis of steroids.

(10Hrs)

## **UNIT IV**

*Plant Pigments. Carotenoids.* Structure and synthesis of  $\beta$ -carotene.

*Flavonoids*. Nature, general methods for structure elucidation and synthesis of anthocyanins and flavones. Structure and synthesis of cyanidin chloride, cyanin, flavone, flavonol and quercetin. Biosynthesis of flavonoids.

Chlorophyll. Chemistry of chlorophyll.

(12Hrs)

## **UNIT V**

Vitamins and Antibiotics. Vitamins. Structure and synthesis of vitamin  $B_1$  (thiamine),  $B_2$  (riboflavin) and  $B_6$  (pyridoxine). Chemistry of Vitamin  $B_{12}$ .

Antibiotics. Structure and synthesis of penicillins and chloramphenicol.

(11Hrs)

- 1. I.L. Finar, Volume 2, ELBS, Essex.
- J. Mann, R.S. Davidson, J.B. Hobbs, D.V. Banthrope and J.B. Harborne, Natural products, chemistry and biological significance, Longman, Essex.

## M.Sc. SEMESTER IV Course 05 (CHE-402B) (ELECTIVE PAPER V): Physical Organic Chemistry

Maximum Marks: 100 (End Sem.:60+CE: 40) Credit: 3

**Teaching Hour: 54** 

#### **UNIT I**

Quantitative Molecular Orbital (MO) Theory. Hückel molecular orbital method as applied to ethene, allyl and butadiene. Qualitative MO theory-ionisation potential. Electron affinities. MO energy levels. Orbital symmetry. Orbital interaction diagrams. MO of simple organic systems such as ethene, allyl, butadiene, methane and methyl group. Conjugation and hyperconjugation. Aromaticity.

Valence bond (VB) configuration mixing diagrams. Relationship between VB configuration mixing and resonance theory. Reaction profiles. Potential energy diagrams.

(11Hrs)

#### **UNIT II**

Acids, Bases, Electrophiles, Nucleophiles and Catalysis. Acid-base dissociation. Electronic and structural effects, acidity and basicity. Acidity functions and their applications. Hard and soft acids and bases. Nucleophilicity scales. Nucleofugacity. The  $\alpha$ -effect. Ambivalent nucleophiles. Acid-base catalysis, specific and general catalysis. Bronsted catalysis. Nucleophilic and electrophilic catalysis. Catalysis by non-covalent binding-micellar catalysis.

(11Hrs)

## **UNIT III**

Radical and Pericyclic Reactivity. Radical stability, polar influences, solvent and steric effects. A curve crossing approach to radical addition, factors effecting barrier heights in additions, regioselectivity in radical reactions.

Reactivity, specificity and periselectivity in pericyclic reactions.

(10Hrs)

## **UNIT IV**

Supramolecular Chemistry. Properties of covalent bonds-bond length, inter-bond angles, force constant, bond and molecular dipole moments. Molecular and bond polarizability, bond dissociation enthalpy, entropy. Intermolecular forces, hydrophobic effects. Electrostatic, induction, dispersion and resonance energy. Magnetic interactions, magnitude of interaction energy, forces between macroscopic bodies, medium effects. Hydrogen bond.

Principles of molecular association and organization as exemplified in biological macromolecules such as enzymes, nucleic acids, membranes and model systems as micelles and vesicles. Molecular receptors and design principles.

(11Hrs)

## **UNIT V**

Redox Reactions by Excited Metal Complex. Energy transfer under conditions of weak interaction and strong interaction-exciplex formation; conditions of the excited states to be useful as redox reactants, excited electron transfer, metal complexes as attractive candidates (2,2'-bipyridine, and 1,10-phenanthroline complexes), illustration of reducing and oxidising character of ruthenium(II)-bipyridyl complex, its comparison with Fe(II)(bipy)<sub>3</sub>; role of spin-orbit coupling, life time of these complexes. Application of redox processes of electronically excited states for catalytic purposes.

(11Hrs)

- 1. Physical Organic Chemistry, Jack Hine, McGraw-Hill.
- 2. Molecular Mechanics, U. Burkert and N.L. Allinger, ACS Monograph.
- 3. Physical Organic Chemistry, N.S. Issacs, ELBS, Longman.
- 4. The Physical Basis of Organic Chemistry, H. Maskill, Oxford University Press.
- 5. Introduction to Theoretical Organic Chemistry and Molecular Modelling, W.B. Smith, VCH.

## M.Sc. SEMESTER IV Course 05 (CHE-402C) (ELECTIVE PAPER V): Environmental Chemistry

Maximum Marks: 100 (End Sem.:60+CE: 40) Credit: 3

**Teaching Hour: 54** 

#### Unit-I

Atmosphere. Atmospheric layers, Vertical temperature profile, heat/radiation budget of the earth atmosphere systems. Properties of troposphere, thermodynamic derivation of lapse rate. Temperature inversion. Calculation of Global mean temperature of the atmosphere. Pressure variation in atmosphere and scale height. Biogeochemical cycles of carbon, nitrogen, sulphure, phosphorus oxygen. Residence times.

Atmospheric Chemistry. Sources of trace atmospheric constituents: nitrogen oxides, sulphure dioxide and other sulphure compounds, carbon oxides, chlorofluorocarbons and other halogen compounds, methane and other hydrocarbons.

*Tropospheric Photochemistry.* Mechanism of Photochemical decomposition of NO2 and formation of ozone. Formation of oxygen atoms, hydroxyl, hydroperoxy and organic radicals and hydrogen peroxide. Reactions of hydroxyl radicals with methane and other organic compounds. Reaction of OH radicals with SO2 and NO2. Formation of Nitrate radical and its reactions. Photochemical smog meteorological conditions and chemistry of its formation.

(11Hrs)

#### **Unit-II**

Air Pollution. Air pollutants and their classifications. Aerosols-sources, size distribution and effect on visibility, climate and health.

Acid Rain. Definition, Acid rain precursors and their aqueous and gas phase atmospheric Oxidation reactions. Damaging effects on aquatic life, plants, buildings and health. Monitoring of SO2 and NOx. Acid rain control strategies.

Stratospheric Ozone Depletion. Mechanism of Ozone formation, Mechanism of catalytic Ozone depletion, Discovery of Antarctic Ozone hole and Role of chemistry and meteorology. Control Strategies.

Green House Effect. Terrestrial and solar radiation Spectra, Major green house gases and their sources and Global warming potentials. Climate change and consequences.

Urban Air Pollution. Exhaust emissions, damaging effects of carbon monoxide. Monitoring of CO. Control strategies.

(11Hrs)

#### **Unit-III**

Aquatic Chemistry and Water Pollution. Redox chemistry in natural waters. Dissolved oxygen, biological oxygen demand, chemical oxygen demand, determination of DO, BOD and COD. Aerobic and anaerobic reactions of organic sulphure and nitrogen compounds in water acid-base chemistry of fresh water and sea water. Aluminum, nitrate and fluoride in water. Petrification. Sources of water pollution. Treatment of waste and sewage. Purification of drinking water, techniques of purification and disinfection.

(11Hrs)

## **Unit IV**

Environmental Toxicology. Toxic heavy metals. Mercury, lead, arsenic and cadmium. Causes of toxicity. Bioaccumulation, sources of heavy metals. Chemical speciation of Hg, Pb, As, and Cd. Biochemical and damaging effects.

Toxic Organic Compound. Pesticides, classification, properties and uses of organochlorine and ionospheres pesticides detection and damaging effects.

Polychlorinated biphenyls. Properties, use and environmental continuation and effects.

Polynuclear Aromatic Hydrocarbons. Source, structures and as pollutants.

(11Hrs)

#### **Unit-V**

Soil and Environmental Disasters. Soil composition, micro and macronutrients, soil pollution by fertilizers, plastic an metals. Methods of re-mediation of soil. Bhopal gas tragedy, Chernobyl, three mile island, Minimtata Disease, Sevoso (Italy), London smog.

(10Hrs)

- 1. Environmental Chemistry, Colin Baird, W.H. Freeman Co. New York, 1998.
- Chemistry of Atmospheres, R.P. Wayne, Oxford.
- 3. Environment Chemistry, A.K. De, Wiley Eastern, 2004.
- 4. Environmental Chemistry, S.E. Manahan, Lewis Publishers.
- 5. Introduction to atmospheric Chemistry, P.V. Hobbs, Cambridge.

## M.Sc. SEMESTER IV Course 05 (CHE-402D) (ELECTIVE PAPER V): Heterocyclic Chemistry

Maximum Marks: 100 (End Sem.:60+CE: 40)

Credit: 3 Teaching Hour: 54

#### Unit I

Nomenclature of Heterocycles. Replacement and systematic nomenclature (HantzsCHC-Widman system) for monocyclic fused and bridged heterocycles.

Aromatic Heterocycles. General chemical behaviour of aromatic heterocycles, classification (structural type), criteria of aromaticity (bond lengths, ring current and chemical shifts in 1H NMRspectra. Empirical resonance energy, delocalization energy and Dewar resonance energy, diamagnetic susceptibility exaltations). Heteroaromatic reactivity and tautomerism in aromatic heterocycles.

(11Hrs)

#### Unit II

Non-aromatic Heterocycles. Strain-bond angle and torsional strains and their consequences in small ring heterocycles. Conformatino of six-membered heterocycles with reference to molecular geometry, barrier to ring inversion, pyramidal inversino and 1,3-diaxial interactino. Atereoelectronic effects anomeric and related effects, Attractive interactions-hydrogen bonding and intermolecular nucleophilic lectrophilic interactions. Heterocyclic Synthesis Princples of heterocyclic synthesis involing cyclization reactions and cycloaddition reactions.

(11Hrs)

#### **Unit III**

*Small Ring Heterocycles.* Three-membered and four-membered heterocycles-synthesis and reactions of azirodines, oxiranes, thiranes, azetidines, oxetanes and thietanes.

Benzo-Fused Five-Membered Heterocycles. Synthesis and reactions including medicinal applications of benzopyrroles, bezofurans and benzothiophenes.

(10Hrs)

#### **Unit IV**

*Meso-ionic Heterocycles.* General classification, chemistry of some important meso-ionic heterocycles of type-A and B and their applications.

Six-Membered Heterocycles with one Heteroatom. Synthesis and reactions of pyrylium salts and pyrones and their comparison with pyridinium & thiopyrylium salts and phridones. Synthesis and reactions of quionlizinium and benzopyrylium salts, coumarins and chromones.

(10Hrs)

## Unit V

Six Membered Heterocycles with Two or More Heteroatoms. Synthesis and reactions of diazones, triazines, tetrazines and thiazines. Seven-and Large-Membered Heterocycles Synthesis and reactions of azepines, oxepines, thiepines, diazepines thiazepines, azocines, diazocines, dioxocines and dithiocines.

Heterocyclic Systems Containing P, As, Sb and B. Heterocyclic rings containing phosphorus. Introduction, nomenclature, synthesis and characteristics of 5- and 6-membered ring systems phosphorinaes, phosphorines, phospholanes and phospholes. Heterocyclic rings containing As and Sb. Introduction, synthesis and characteristics of 5- and 6-membered ring system. Heterocyclic rings containing B. Introduction, synthesis reactivity and spectral characteristics of 3- 5- and 6- membered ring system.

(12Hrs)

- 1. Heterocyclic Chemistry Vol. 1-3, R.R. Gupta, M. Kumar and V.Gupta, Springer Verlag.
- 2. The Chemistry of Heterocycles, T. Eicher and S. Hauptmann, Thieme.
- 3. Heterocyclic chemistry J.A. Joule, K. Mills and G.F. Smith, Chapman and Hall.
- Heterocyclic Chemistry, T.L. Gilchrist, Longman Scietific Techinal.
- Contemporary Hetrocyclic Chemistry, G, R. Newkome and W.W. Paudler, Wiley-Inter Science.
- 6. An Introductiion to the Heterocyclic Compounds, R.M. Acheson, Johnwiely.

7. Comprehensive Heterocyclic Chemistry, A.R. Katrizky and C.W. Rees, eds. Pergamon Press.

## M.Sc. SEMESTER IV LABORATORY COURSE 06-08 (CHC-404-406)

Emphasis should be placed on physical principles, reaction chemistry and the technique involved in experiments. Attention should be placed on stoichiometric calculations and statistical analysis of results. In regular classes, each student should perform all the experiments as selected by the Department from the list in the syllabus. In examination, students should be given different experiments or combination of experiments.

| Course | 06 (CHC 404): Inorganic Chemistry (6 hours; 1 day) | End Sem. +CE<br>60+40=100 | Credit 3 |
|--------|--|---------------------------|----------|
|        | Record +Viva voce + Attendance                     | 5+5+5=15                  |          |
|        | Two or three Experiments based on the following:   | 45                        |          |
| (a)    | Spectrophotometric                                 |                           |          |
| (b)    | Cyclic voltammetric                                |                           |          |
| (c)    | Spectral analysis                                  |                           |          |

| (iii) Course 07 (CHC-405): Organic Chemistry (6 hours; 1 day) |  | End Sem. +CE<br>60+40=100 | Credit 3 |
|---|--|---------------------------|----------|
|   | Record +Viva voce + Attendance                   | 5+5+5=15                  |          |
|   | Two or three Experiments based on the following: | 45                        |          |
| (a)   | Synthesis  |                           |          |
| (b)   | Quantitative                                     |                           |          |
| (c)   | Spectral analysis                                |                           | ·        |

| (iii) Cour | se 08 (CHC-406): Physical Chemistry (6 hours; 1 day) | End Sem. +CE<br>60+40=100 | Credit 3 |
|------------|--|---------------------------|----------|
|            | Record +Viva voce + Attendance                       | 5+5+5=15                  |          |
|            | Two Experiments based on the following:              | 45                        |          |
| (a)        | Chemical Kinetics                                    |                           |          |
| (b)        | Spectrophotometric                                   |                           |          |
| (c)        | Electronics  |                           |          |
| _          |  |                           |          |

| Compressive Viva voce | Max. Marks 50 | Credit 4* |
|-----------------------|---------------|-----------|
|-----------------------|---------------|-----------|

#### Course 06 (CHC-406): Inorganic Chemistry

Sectrophotometric Determination

- Determination of molecular composition of ferric salicilate /iron-phenanthroline/iron-dipyridyl complex by Job's method of continuous variation
- 2. Stability constant of FeSCN<sup>2+</sup> complex
- 3. Determination of the pH of a given solution by spectrophotometry using methyl red indicator

## Model Experiments on Cyclic Voltammetry

Acquaintance with cyclic voltammetry experiments involving use of K<sub>3</sub>[Fe(CN)<sub>6</sub>]

- 1. Cyclic voltammograms of K<sub>3</sub>[Fe(CN)<sub>6</sub>] at different scan rates
- 2. Cyclic voltammograms of K<sub>3</sub>[Fe(CN)<sub>6</sub>] at different concentrations

Interpretation of ESR, NMR and Thermogravimetric pre-recorded results of known compounds

Pre-recorded spectrum/data shall be provided for their interpretation leading to structure determination of metal ion complexes with organic ligands.

## Course 07 (CHC-407): Organic Chemistry

Multi-step Synthesis

Heterocyclic compounds

Phenylhydrazine  $\rightarrow$  acetophenone phenylhydrazone  $\rightarrow$  2-phenylindole

Quinoline from Skraup synthesis

Ethyl acetoacetate → 3-methyl-1-phenylpyrazol-5-one → antipyrin (phenazone)

Benzaldehyde  $\rightarrow$  benzoin  $\rightarrow$  benzil  $\rightarrow$  5,5-diphenylhydantoin

Benzaldehyde  $\rightarrow$  benzoin  $\rightarrow$  benzil  $\rightarrow$  2,3-diphenylquinoxaline

### Mixed principles

Aniline  $\rightarrow$  2,4,6-tribromoaniline  $\rightarrow$  1,3,5-tribromobenzene

Aniline  $\rightarrow$  2,4,6-tribromoaniline  $\rightarrow$  2,4,6-tribromo-1-chlorobenzene

Phenol  $\rightarrow$  mixture of 2- and 4- nitrophenols  $\rightarrow$  separate 2- and 4- nitrophenols

Chlorobenzene  $\rightarrow$  1-chloro-2,4-dinitrobenzene  $\rightarrow$  2,4-dinitrophenylhydrazine

#### Quantitative Analysis

Determination of methoxy group

Determination of halogen by fusion or oxygen flask combustion method

Diol groups (ring size in carbohydrates) by periodate oxidation

Spectrophotometric (colorimetric) determination of glucose by Fehling reaction

Determination of acetone by iodoform reaction

Determination of vitamin C in drug formulations and in fruits

### Spectral Analysis

Interpretation of pre-recorded UV-Vis, IR, NMR, Mass, Raman spectrum and characterisation of one organic compound.

## Course 08 (CHC-408): Physical Chemistry

## Spectrophotometry

1. Determination of stability constant of Fe(III)-salicyclic acid complex

#### Chemical Kinetics

- 2. Determination of order of  $S_2O_8^{2-}$ — $I^-$  reaction
- 3. Determination of energy of activation of  $S_2O_8^2$ —I reaction
- 4. Studies on the effect of variation of ionic strength on the rate of  $S_2O_8^2$ — $I^2$  reaction
- 5. Ester hydrolysis catalysed by a base
- 6. Kinetics of acid-catalysed reaction between acetone-iodine

## Electronics

- 7. Voltage measurement with CRO
- 8. Measurement of e.m.f. with thermocouple
- 9. To plot the characteristic curve of a diode

- 1. Vogel's Textbook of Quantitative Analysis, revised, J. Bassett, R. C. Denney, G. H. Jeffery and J. Mendham, ELBS.
- 2. Analytical Chemistry, S.M. Khopkar, New Age International Ltd., New Delhi.
- 3. Synthesis and Characterization of Inorganic Compounds, W. L. Jolly, Prentice Hall
- 4. Experiments and Techniques in Organic Chemistry, D. Pasto, C. Johnson and M. Miller, Prentice Hall
- 5. Macroscale and Microscale Organic Experiments, K. L. Williamson, D. C. Heath.
- 6. Systematic Qualitative Organic Analysis, H. Middleton, Adward Arnold.
- 7. Handbook of Organic Analysis- Qualitative and Quantitative, H. Clarke, Adward Arnold.
- 8. Vogel's Textbook of Practical Organic Chemistry, ELBS.
- 9. F.G. Mann and B.C. Saunders, Practical Organic Chemistry, Orient Longman.
- 10. Findley's Practical Physical Chemistry, B. P. Levitt, Longman
- 11. Experimental Physical Chemistry, R.C. Das and B. Behera, Tata McGraw Hill.
- 12. Practical Physical Chemistry, A. M. James and F. E. Prichard, Longman