# FOR M.Sc. Chemistry

(CBCS-Based)

\$55° \$

# CBCS-based syllabus for M.Sc. Chemistry (2 years) Programme

# **General Informations:**

- (1) It is two years Master Degree Programme
- (2) There shall be four semester to complete programme, i.e. 1st, 2nd, 3rd and 4th semester
- (3) Each semester shall consist of 15 weeks of academic work equivalent to 90 actual teaching days.
- (4) This programme will have three types of courses, i.e. Core course and Elective course.

<u>Core course-</u> The core courses are those courses whose knowledge is deemed essential for the students registered for a particular Master's degree programme.

Elective course. The elective course can be choosen from a pool of papers in II<sup>nd</sup> and IVth semester.

- (5) Each course will have 100 marks in full and divided into 70 marks for end-semester exam and 30 marks for internal assessment work except AEC, AECC-1, AECC-2 and practical papers. Internal assessment will be in two internal exams of 10 marks each, 5 marks for seminar/internal project and 5 marks for attendance/discipline.
- (6) In practical papers the distribution of marks in CIA will be same as prescribed for term end semester practical papers.
- (7) A student in fourth semester can choose a generic paper or CC-5 paper of any other subject of the faculty as DSE.

<u>Credits-</u> A unit by which the course work is measured. It determines the number of hours of instruction required per week. One credit is equivalent to one hour of teaching (lecture or tutorial) or two hours of practical work/ field work per week.

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# M.Sc. Chemistry (Two years Course) CHOICE BASED CREDIT SYSTEM

#### Course Structure

# M.Sc. Ist Semester

| Serial<br>No. | Courses            | Code        | Description  | Credits | Max.<br>Marks<br>(100) |
|---------------|--------------------|-------------|--|---------|------------------------|
| 1             | Core Course<br>I   | MSCCHE CC-1 | Inorganic Chemistry-1  | 5       | 100                    |
| 2             | Core Course<br>II  | MSCCHE CC-2 | Physical Chemistry-1   | 5       | 100                    |
| 3             | Core Course<br>III | MSCCHE CC-3 | Organic Chemistry-1  | 5       | 100                    |
| 4             | Core Course<br>IV  | MSCCHE CC-4 | Practical (Physical)   | 5       | 50750<br>70 +30        |
| 5             | AECC-1             |             | Environmental Sustainability and Swachchchha Bharat Abhiyan Activities | 3+2     | 50+50                  |

# M.Sc. II<sup>nd</sup> Semester

| Serial<br>No. | Courses             | Code        | Description            | Credits | Max.<br>Marks<br>(100)               |
|---------------|---------------------|-------------|------------------------|---------|--------------------------------------|
| 6             | Core Course<br>V    | MSCCHE CC-5 | Advances in Chemistry  | 5       | 100                                  |
| 7             | Core Course<br>VI   | MSCCHE CC-6 | Inorganic Chemistry-II | 5       | 100                                  |
| 8             | Core Course<br>VII  | MSCCHE CC-7 | Physical Chemistry-II  | 5       | 100                                  |
| 9             | Core Course<br>VIII | MSCCHE CC-8 | Organic Chemistry-II   | 5       | 100                                  |
| 10            | Core Course<br>IX   | MSCCHE CC-9 | Practical (Organic)    | 5       | <del>50+50</del><br><del>70+30</del> |
| 11            | AEC-1               | -           |                        | 5       | 50+50                                |

# M.Sc. III<sup>rd</sup> Semester

| Serial<br>No. | Courses             | Code         | Description   | Credits | Max.<br>Marks<br>(100) |
|---------------|---------------------|--------------|---|---------|------------------------|
| 12            | Core Course<br>X    | MSCCHE CC-10 | Application of Spectroscopy                                 | 5       | 100                    |
| 13            | Core Course<br>XI   | MSCCHE CC-11 | Bio-inorganic Chemistry                                     | 5       | 100                    |
| 14            | Core Course<br>XII  | MSCCHE CC-12 | Environmental Chemistry and Green Chemistry                 | 5       | 100                    |
| 15            | Core Course<br>XIII | MSCCHE CC-13 | Bio-organic Chemistry                                       | 5       | 100                    |
| 16            | Core Course<br>XIV  | MSCCHE CC-14 | Practical (Inorganic<br>Chemistry)                          | 5       | 50+50<br>70+30         |
| 17            | AECC-2              |              | Human values and professional ethics & Gender sensitization | 3+2     | 50+50                  |

# M.Sc. IV<sup>th</sup> Semester

| Serial<br>No. | Courses              | Code         | Description                              | Credits | Max.<br>Marks<br>(100) |
|---------------|----------------------|--------------|--|---------|------------------------|
| 18            | Elective<br>Course-1 | MSCCHE EC-1a | Inorganic Chemistry Special              | 5       | 100                    |
| 19            | Elective<br>Course-1 | MSCCHE EC-1b | Physical Chemistry Special               | 5       | 100                    |
| 20            | Elective<br>Course-1 | MSCCHE EC-1c | Organic Chemistry Special                | 5       | 100                    |
| 21            | Elective<br>Course-2 | MSCCHE EC-2a | Inorganic Chemistry Special<br>Practical | 5       | 50+50<br>70+30         |
| 22            | Elective<br>Course-2 | MSCCHE EC-2b | Physical Chemistry Special<br>Practical  | 5       | 50+50<br>70+30         |
| 23            | Elective<br>Course-2 | MSCCHE EC-2c | Organic Chemistry Special<br>Practical   | 5       | 50+50<br>70+30         |
| 24            | DSE-1 or<br>GE-1     |              |  | 5       | 100                    |

Candidates should choose any one among the following groups- 1a & 2a or 1b & 2b or 1c & 2c

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# Semester- I Core Course – I Inorganic I

Full Marks – 70 Credits- 5

Unit-I (a) VSEPR theory,  $d\pi$ -p $\pi$  bonding, Bent rule and energetic of hybridisation.

(b) M.O. diagram for hetero-nuclear di-molecules.

# Unit- II Magnetochemistry

Term symbols, ground state and all possible term, symbols for  $p^2$  and  $d^2$  configuration, quenching of orbital contribution in metal complexes, magnetic properties of inner transition metals, anomalous magnetic behavior of  $E_u^{3+}$  and Sm3+ ions.

Unit- III Metal-Ligand Equilibrium in Solution

Stepwise and overall formation constants and their interaction, trends in stepwise constants, factors affecting the stability of metal complexes with reference to the nature of metal ion and ligand, cheiate effect and its thermodynamic origin.

Unit - IV Reaction Mechanism of Transition metal complexes.

Inert and labile complexes, kinetic application of VBT and CFT, kinitics of octahedral substitution, acid hydrolysis, base hydrolysis, CB mechanism, Evidences of CB mechanism, Anation reaction, reaction without M.L bond cleavage, substitution reactions in square, lanar occuplexes. The transeffect, Theories of trans-effect.

Unit - V Isopoly and Heteropoly Acids and salts, Isopoly and Heteropoly acids and salts of Mo and W. structure of isopoly and heteropoly anions.

#### Books Recommended

- 1. Concise Inorganic Chemistry- J.D. Lee
- 2. Inorganic Chemistry- T. Moeller.
- 3. Modern Aspects of Inorganic Chemistry- H.J. Emeleus and A.G. Sharpe

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- 4. Introduction to ligand field- B.N. Figgis
- 5. Inorganic Reaction Mechanism- Basalo and Pearson
- 6. Chemical bonding- O.P. Agrawal
- 7. Structural Principles in Inorganic Chemistry- W.E. Addison.
- 8. Introduction the Magneto Chemistry- A. Earnshasw

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#### Semester- I

#### Core Course - II

#### Physical Chemistry-I

Full Marks-70

Credits-5

#### Unit- I Macromolecules

Types of polymers, Kinetic and machanisms of polymerization, Molar mass, number and mass average molar mases, determinations of molar mass by osmometry, viscometric and light scattering method.

# Unit- II Electro Chemistry

- (i) Electrode potential in terms of Chemical Potential and activity.
- (ii) Debye Huckel theory of conductance of electrolytic solution, its application and limitations.
- (iii) Quantitative treatment of Debye Huckel Limiting law and its modification for finite size of ions, effect of ion solvent interaction on activity coefficients.
- (iv) Butle-Volmer equation under equilibrium and non equilibrium condition. Exchange current density Tafel Plot.

# Unit- III Chemical Dynamics

- (a) Machanism and Dynamics of consecutive and opposing reactions.
- (b) Activated complex theory of reaction rate, Evalution of free anergy, enthalpy and entropy of activation.
- (c) Mechanism and dynamics of Photolysis of acetaldehyde and photo dimerisation of Anthracene, Polymerization and Auto oxidation reaction.
- (d) Homogeneous catalysis, Kinetics of Enzyme catalysis, study of fast reactions by flow method and relaxation method.

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# Unit- IV Chemical Thermodynamics

- (a) Partial molar properties in ideal mixture, Chemical Potential, its determination and variation with temperature and pressure, Gibbs Duhem equation.
- (b) Fugacity and activity its variation with temperature and pressure, its determination of fugacity of a gas in mixture, Duhem. Margules equation and its application.

# Unit- V Statistical Thermodynamics

Ensembles, Thermodynamic probability, Boltzman Distribution Law, Boltzman Planck Equation, Partition function and its significance, Relationship with thermodynamic functions, Translational, Rotational, Vibrational and Electronic partition function. Its application in the case of monatomic and diatomic molecules, Sackur-Tetrode Equation.

# **Books Suggested:**

1. Physical Chemistry : P.W. Atkins (ELBS)

2. Comprehensive Physical Chemistry : Hemant Snehil

3. Theoretical Physical Chemistry : Gladstone.

4. Physical Chemistry : G.M. Barrow.

5. Modern Electrochemistry : JOM Bakris and A.K.N. Reddy

6. Text Books of Polymer Science : F.W. Billmayer Jr.

7. Advanced Physical Chemistry : Gurdeep Raj

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#### Semester- I

#### Core Course- III

#### Organic Chemistry- I

Full Marks - 70

Credits-5

# Unit- I Nature of Bonding in Organic Molecules

Delocalized chemical bonding conjugation, cross conjugation, resonance, hyperconjugation, Aromaticity in benzenoid and non-benzenoid compounds, Huckel's rule, energy level of  $\pi$ -molecular orbitals, annulenes, antiaromaticity, homo-aromaticity, PMO approach.

# Unit- II Stereochemistry:

Chirality, elements of symmetry, molecules with more than one chiral centre, diastereomerism. Determination of relative and absolute configuration, Methods of resolution, optical purity, conformational analysis of cycloalkanes (six membered rings), decalins, Effect of conformation on reactivity, optical activity in absence of chiral carbon (biphenyls, allenes and spiranes), chirality due to helical shape, stereospecific and stereoselective synthesis.

# Unit- III Reaction Mechanism: Structure and Reactivity:

Types of reactions, kinetic and thermodynamic control, Hammond's postulate. Potential energy diagrams, transition states and intermediates, methods of determining mechanisms, isotope effects. Generation, structure, stability and reactivity of carbocations, carbanions, free radicals, carbenes

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and nitrenes. Effect of structure on reactivity. The Hammett equation and linear free energy relationship, substituent and reaction constants.

# Unit- IV Aliphatic Nucleophilic Substitution:

The  $SN^2$ ,  $SN^1$ , mixed  $SN^1$  and  $SN^2$ ,  $SN^i$  mechanisms. The neighbouring group participation by  $\pi$  and  $\sigma$  bonds. Classical and nonclassical carbocations, phenonium ions, Reactivity- effects of substrate structure, attacking nucleophile, leaving group and reaction medium. Ambident nucleophiles and regioselectivity. Nucleophilic substitution at an allylic, aliphatic trigonal and a vinylic carbon.

**Aromatic Nucleophilic Substitution:** The ArSN<sup>1</sup>, ArSN<sup>2</sup>, Benzyne and SRN<sup>1</sup> mechanisms. Reactivity – effect of substrate structure, leaving group and attacking nucleophile. Von- Richter, Sommelet-Hauser, and Smiles rearrangements.

Unit-V Free radical Substitution: Allylic halogenation, arylation of aromatic componds, Sandmeyer reaction, Hunsdiecker reaction.

Aromatic Electrophilic Substitution: The arenium ion mechanism, orientation and reactivity, energy profile diagrams. The ortho/para ratio, Diazonium coupling, Vilsmeir reaction, Gattermann-Koch reaction.

**Elimination Reactions:** The E2, E1 and E1CB mechanisms. Orientation of the double bond. Stereochemistry of E2 reaction, Hofmann's rule and Saytzeff's rule.

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#### **Books Recommendation:**

- Advanced Organic Chemistry- Reactions Mechanism and Structure by Jerry March.
- 2. A guide Book to Mechanism in Organic Chemistry by Peter Sykes.
- 3. Organic Chemistry by R.T. Morrison and R.N.Boyd.
- 4. Advanced Organic Chemistry by Jagdamba Singh and L. D. S. Yadav.
- 5. Reaction Mechanism in Organic Chemistry by S.M. Mukherji and S.P. Singh.
- 6. Stereochemistry of Organic Compounds by D. Nasipuri.
- 7. Stereochemistry of Organic Compounds by P.S. Kalsi.
- 8. Advanced Organic Chemistry by F.A. Carey and R.J. Sundberg.
- 9. Organic Synthesis by Jagdamba Singh, L. D. S. Yadav and Jaya singh.

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#### Semester- I

# **Practical (Physical Chemistry)**

#### (Core Course- IV)

Full Marks- 50 Credits-5

# Any one experiment- 30 Marks

- 1. Water equivalent of calorimeter and determination of
  - (i) Heat of solution of potassium nitrate
  - (ii) Heat of neutralization of strong acid and strong base.
  - (iii) Basicity of polybasic acids.
- 2. Determination of rate constant of hydrolysis of methyl acetate in acid medium.
- 3. The study of saponification of ethyl acetate by sodium hydroxide and determination of rate constant.
- 4. To determine the distribution coefficient of
  - (i) Acetic acid
  - (ii) Benzoic acid

    Between water and benzene by partition method.
- 5. Determination of specific and molar rotation of sucrose in different concentrations and to determine the concentration of given solution.
- 6. Determination of rate constant by inversion of cane sugar by Polarimetrically
- 7. Determination of
  - (i) Dissociation constant of acetic acid.
  - (ii) Acid-base titration.
  - (iii) Solubility product of sparingly soluble salt.

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# Semester- II Core Course – V Advances in Chemistry

# Unit- I Nuclear Chemistry

- (a) Shell model, Liquid Drop Model, Nuclear Reactions and their Types.

  Nuclear Reaction Cross-section.
- (b) Application of radio isotopes, tracer Techniques, Neutron activation analysis, isotope dilution method, Nuclear reactor.

# Unit- II Nanomaterials and Green chemistory

Definition, sources, examples, Bottom-up Method of synthesis, Characterizations, and applications, synthesis in green chemistory.

# Unit- III Solid State Chemistry

Conductor, Semiconductor, and superconductor; Theory and Applications

# Unit- IV Industrial Application of Chemistry

Chemistry of Cement, Paper and Pulp, and Petroleum

# Unit- V Waste Management

Nuclear waste management, e-waste management,

Recycling of plastic: sorting, washing, shredding, identification and classification, extruding.

# Semester- II Core Course – VI Inorganic Chemistry II

Full Marks – 70 Credits- 5

# Unit- I Electronic Spectra of Transition Metal Complexes.

Spectroscopic ground states, correlation and spin-orbit coupling in free ions for 1<sup>st</sup> series of transition metals, Orgel and Tanabe-Sugano diagrams for transition metal complexes (d¹-d9 states), calculation of Dq, B and β parameters, effect of distortion on the d-orbital energy levels. Structural evidence from electronic spectrum, John-Tellar effect, Spectrochemical and nephalauxetic series, charge transfer spectra, electronic spectra of molecular addition compounds.

# Unit- II Symmetry in Chemistry.

Symmetry elements and symmetry operations, definition of groups, subgroup, conjugate and class. Point symmetry group. Requirements of a mathematical group, multiplication table for  $C_{2V}$ ,  $C_{3V}$ 

# Unit- III Group theory in Chemistry.

Representation of group by matrices. Working out representation of  $C_{2V}$ ,  $C_{3V}$  point groups. Character of a representation. The great orthogonality theorem (without proof) and its importance in derivation of character table. Construction of character table for  $C_{2V}$  and  $C_{3v}$  point group.

# Unit – IV Metal *n*-complexes.

Metal carbonyls, structure and bonding, vibrational spectra of metal carbonyls for bonding and structural elucidation. Preparation, bonding, structure and important reaction of transition metal nitrosyls.

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# Unit- V Metal Clusters

Structure and bonding in higher boranes, Wade's rules, Carboranes.

# **Books Recommended:**

- 1. Advanced Inorganic Chemistry- F.A. Cotton and G. Wilkinson.
- 2. Inorganic Chemistry- Principles of Structure and reactivity J.E. Huheey
- 3. Concise Inorganic Chemistry- J.D. Lee
- 4. Group Theory and its chemical applications- F.A. Cotton
- 5. Group Theory and its chemical applications- P.K. Bhattacharya

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#### Semester-II

#### Core Course - VII

# Physical Chemistry-II

Full Marks- 70 Credits- 5

# Unit- I Introduction of quantum mechanics

- (i) Functions and operators and their types and properties, Dirac's Braket notation, normalisation and orthogonalisation of functions, Kronecker delta.
- (ii) Quantum mechanical operators and physical quantities, Time dependant and time independant schrodinger wave equations, Expection values.

# **Unit-II** Exactly Soluble System.

- (i) Linear Harmonic oscillator, Harmonic Vibration, Hermite differential equation and its solution through recursion relation. Hermite polynomial.
- (ii) H-like atoms, separation of R(r), Θ(θ) and Φ (φ) Equations and their solutions, radial and angular wave functions, radial distribution functions, Laguerre and Associated Laguerre Polynomials, Legendre polynomials and Associated Legendre polynomials, quantam mechanical treatment of rigid rotator.

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# Unit- III Approximate Method.

Variation method, Secular equation, Perturbation method, first order perturbation, Application to He-atom. Symmetric and antisymmetric wave functions. Slater determinant, singlet and triplet states.

# Unit- IV Chemical Bonding

Born Oppenheimer approximation, LCAO-MO theory, application of LCAO-MO theory to H<sub>2</sub><sup>+</sup> ion and H<sub>2</sub> molecule, V.B. theory and it's application to H<sub>2</sub> molecule

# Unit-V Huckel Molecular Orbital Theory

Huckel theory of conjugated systems, Application to ethylene, butadiene, allyl systems and benzene, calculation of D.E.,  $\pi$ -electron density and  $\pi$ -bond order.

# **Books Suggested:**

1. Quantum Chemistry : I.R. Lavine Prentiee Hall.

2. Quantum Chemistry : Pillar

3. Quantum Chemistry : R.K. Prasad

4. Ouantum Chemistry : Satya Prakash Swati Saluja

5. Solid State Chemistry : D.K. Chakrabarty, New Age International

6. New Direction Solid

State Chemistry : C.N. R. Rao & J. Gopal

7. Introduction to quantum : A.K. Chandra, Tata

8. Quantum Chemistory : A.B. Sannigrahi

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# Semester- II Core Course- VIII Organic Chemistry- II

Full Marks – 70 Credits- 5

#### **Unit- I** Addition to Carbon-Carbon Multiple Bonds:

Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, regio –selectivity, orientation and reactivity. Hydrogenation, Hydroxylation Hydroboration.

Michael reaction.

# Addition to Carbon-Hetero Atom Multiple Bonds:

Nucleophilic addition of carbonyl compounds,

Mechanism of metal hydride reduction of saturated carbonyl compounds, Wittig reaction. Mechanism of condensation reactions involving enolates – Aldol, Benzoin, Perkin and Stobbe reactions.

# **Unit-II** Photochemistry of Carbonyl Compounds:

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Principles of Photochemistry, Electronic excitation, hydrogen abstraction. photochemistry of p-benzophenones, Norrish type I and Norrish type II, reaction, Paterno-Buchi reaction.

#### Photochemistry of unsaturated system

Olefins, cis-trans isomerisation, dimerisation, hydrogen abstraction and additions. photochemistry of 1, 3-butadiene (2+2) additions leading to cage structures, photochemistry of cyclohexadienes, Photo-Fries rearrangement, Photo-Fries reaction of anilides, photosubstitution reaction of benzene derivatives, Photolysis of nitride esters and Barton reaction.

#### Unit- III Pericyclic Reactions

Molecular orbital symmetry, Frontier orbitals of ethylene, 1, 3-butadiene, 1,3,5-hexatriene and allyl system, Classification of pericyclic reactions, Woodward-Hoffmann principle FMO and PMO approach, Electrocyclic reactions-conrotatory and disrotatory motions, 4n, 4n+2 and allyl systems. Cycloadditions-antrafacial and suprafacial additions, 4n and 4n+2 systems, 2+2 addition of ketenes, 1,3-dipolar cycloadditions and

#### Sigmatropic rearrangement

Suprafacial and antarafacial shift of H, sigmatropic shifts involving carbon moieties, (3,3) and (5,5) sigmatropic rearrangements, detailed treatment of Claisen and Cope-rearrangements. Introduction to Ene reactins.

#### Unit- IV Oxidation:

Different oxidative processes, oxidation of alkenes, aromatic rings, alcohols, diols, ketones with emphasis on oxidation by peracides, peroxides, HIO<sub>4</sub>, Pb(OAc)<sub>4</sub> and SeO<sub>2</sub>.

# Unit-V Molecular rearrangements

General mechanistic consideration, A detail study of the following rearrangements: Wegner-Meerwein rearrangements Neber, Curtius, Arndt Eistert reaction, Benzilic acid, Beckmann rearrangements.

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# **Books Recommended**

- 1. Structure and Mechanism in Organic Chemistry by C.K. Ingold.
- 2. Modern Organic Reactions by H.O. House .
- 3. Principles of Organic Synthesis by R.O.C. Norman and J.M. Coxon.
- 4. Reaction Mechanism in Organic Chemistry by S.M. Mukherji and S.P. Singh.
- 5. Carbohydrate by S.P. Bhutani.
- 6. Organic Chemistry by I.L. Finar.
- 7. Photochemistry and Pericyclic reactions by Jagdamba Singh and Jaya singh.
- 8. Introductory Photochemistry by A. Cox and T. Camp.
- 9. Photochemistry by R.P. Kundall and A. Gilbert.
- 10. Organic Photochemistry by J. Coxon and B. Halton.
- 11. Organic Photochemistry by Orville L. Chapman.
- 12. Pericyclic Reactions by S.M. Mukherji.
- 13. The Conservation of Orbital Symmetry by R.B. Woodward and R. Hoffman.
- 14. Orbital Symmetry by R.E. Lehr and A.P. Merchant.

#### Semester- II

#### Core Course- IX

#### Practical (Organic Chemistry)

Full Marks- 50 Credits- 5

#### 1. Quantitative Analysis

Separation and identification of organic compounds in binary mixtures by chemical tests and preparation of their derivatives.

15 Marks

# 2. Organic Synthesis via two steps preparation

15 Marks

- a. p-Nitroaniline from acetanilide.
- b. p-Bromoaniline from acetanilide
- c. Anthranilic acid from phthalic anhydride.
- d. p-Bromoacetanilide from aniline.
- e. p-Nitroacetanilide from aniline.

3. Viva Voce 15 Marks

4. Note Book 05 Marks

#### **Books Recommendation:**

- 1. Advanced Practical Chemistry by Jagdamba Singh, L. D. S. Yadav and Jaya singh
- 2. Systematic Qualitative Organic Analysis by H. Middleton .
- 3. Handbook of Organic Analysis-Qualitative and Quantitative by H. Clark.
- 4. Vogel's Textbook of Practical Organic Chemistry by A. R. Tatchell.

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# Semester- III Core Course- X Application of Spectroscopy

Full Marks-70

Credits - 5

#### **Inorganic Spectroscopy**

#### Unit- I(A) Rotational Spectroscopy

Quantization of rotational energy and interactions of radiation with rotators. Classification of rotators; rigid rotator and Non-rigid rotator linears, Symmetric top, symmetric and asymmetric rotators, isotopic effect, starck effect, effect of nuclear spin, and electron spin on rotational spectra.

#### (B) Applications -

Determination of internuclear distance of diatomic molecule, dipolemoment, atomic mass of isotope, effect of bond distortion on rotational energies.

# Unit- II (A) Vibrational Spectra

Harmonic oscillator model, harmonic and anharmonic vibration, Normal vibration, Factors affecting vibration frequencies, vibrating rotators, P.Q.R. Branches, overtones, anharmonicity constant, Raman effect, stokes and antistokes lines, selection rules for IR and Raman spectra, Principle of mutual exclusion. Polarization of Raman Lines.

# (B) Applications-

Organic effect of conjugation, resonance inductive effect, ring strain and hydrogen bonding on group frequencies and band shapes.

Inorganic: Changes with vibrational frequencies upon co-ordination, cases of linkage isomers, I.R. and Raman active form of vibrational geometry of AB<sub>2</sub>, AB<sub>3</sub>, AB<sub>4</sub> and AB<sub>5</sub>. Hydrogen bonding.

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# Unit- III (A) Magnetic Resonance Spectroscopy

Nuclear magnetic resonance, chemical shift, factors controlling its value spin-spin interaction and factors affecting its value. Spin Lattice relaxation and quantative treatment of relaxation, selection rule and relative intensities of line. Principle of ESR spectroscopy, presentation of spectrum, theory of hyperfine, interaction, Isotopic g and  $\Delta$  values.

# (B) PMR and CMR Spectroscopy

Chemical shifts value and correlation for proton-bonded with carbon. Effect of chemical exchange on line width, coupling constants, Interpretation of PMR and CMR spectra of organic compounds. Double resonance application of <sup>19</sup>F and <sup>31</sup>P spectra of inorganic compounds.

# Unit- IV (A) Mass Spectrometry

Ion production and Fragmentation, molecular ion peak, Metastable peak, Mc. Lafferty rearrangement. Examples of mass spectra of organic compounds.

(B) Basic principles, spectral parameters and spectrum display, Application of the technique to the studies of (1) bonding and structure of Fe<sup>+2</sup> and Fe<sup>+3</sup> compounds including those of intermediates spin. (2) Sn<sup>+2</sup> and Sn<sup>+4</sup>

#### Unit- V

# (A) UV-Visible Spectroscopy

Spectra of carbonyl compounds and conjugated polyenes, Woodward-Fisher rules, aromatic and heterocyclic compounds, and steric effect in diphenyls, quantitative determinations.

# (B) Photoelectron Spectroscopy

Basic principles of photoelectric effect ionization. Process, PES and XPS photo-electron spectra of O<sub>2</sub>, N<sub>2</sub> and NO (simple molecule). Adiabatic and vertical ionization energy, Koopman's theorem.

#### **Book Suggested**

- 1. Physical Methods for Chemistry by R.S. Drago, Saunders Company.
- 2. Structural Methods in Inorganic Chemistry by E.A.V. Ebsworth, D.W.H. Rankin and S. Cradock, ELBS.
- 3. Infrared and Raman Spectra: Inorganic and Co-ordination Compounds by K. Nakamoto, Wiley.
- 4. Progress in Inorganic Chemistry Vol. 8, ed by F.A. Cotton, Vol. 15, ed, S.J. Lipard, Wiley.
- 5. Inorganic Electronic Spectroscopy by A.P.B. Lever, Elsevier.
- 6. Organic Spectroscopy by Jagdamba Singh and Jaya singh.
- 7. Spectroscopy of Organic Compounds by P S Kalsi.
- 8. Spectrometric identification of organic compounds by Silverstein.

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#### Semester-III

#### Core Course- XI

#### **Bio-Inorganic Chemistry**

Full Marks - 70

Credits-5

# Unit- I Metal Ions in Biological Systems

Essential and trace metals. Role of metals ions (Ca,Mg,Na,K) in biological processes. Toxicity of heavy metals and their detoxification, role of Selenium in Biological systems with reference to its essentiality and toxicity, mechanism of metal ion induced toxicity.

# Unit- II Bioenergetics and ATP Cycle

DNA polymerization, metal complexes in transmission of energy, chlorophylls, photosystem I and photosystem II in cleavage of water system.

#### Unit- III. Transport and Storage of Dioxygen

Structure and function of haemoglobin, myoglobin, hemicyanics model synthetic complexes of iron, cobalt and copper.

# Unit- IV Electron Transfer in Biology

Structure and function of metalloproteins in electron transport processes – cytochromes and ion-sulphur proteins, synthetic models.

#### Nitrogenase

Biological nitrogen fixation, molybdenum nitrogenase, spectroscopic and other evidence, other nitrogenases model system.

#### Unit- V Metals in Medicine

Biochemical bases of essential metal deficient diseases; Iron, copper and zinc deficiencies and their therapies, carcinogens and

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carcinostatic agents, zinc in tumour growth and inhibition, anticancer activity and mechanism of platinum complexes, anticancer activity of Rhodium, copper and Gold complexes, anticancer activity of Selenium, antibacterial and antiviral properties of metal complexes.

#### **Books Recommend:**

- 1. Principles of Bio-inorganic Chemistry- S.J. Lippard and J.M. Berg, University Science Books.
- 2. Bio-inorganic Chemistry- I. Bertini, H.B. Gray, S.J. Lippard and J.S. Valentine, University Science Books
- 3. Progress in Inorganic Chemistry, Vols 18 and 3S Ed. J.J. Lippard, Wiley.

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# Semester- III Core Course- XII (Environmental Chemistry and Green Chemistry)

Full Marks-70

Credits - 5

#### **Unit-I Environment**

Introduction, Composition of atmosphere, vertical temperature, heat budget of the earth atmospheric system, vertical stability atmosphere, Biogeochemical cycles of C, N, P, S and O. bio distribution of elements.

#### Unit -II Hydrosphere

Chemicals compositions of water bodies-lakes, streams, rivers, and wet lands etc. hydrological cycle, Aquatic Pollution – inorganic, organic, pesticide, agricultural, industrial and sewage, detergents, oil spills and oil pollutants. Water quality parameters – dissolved oxygen, biochemical oxygen demand (BOD), Solids, metals, content of chloride, sulphate, phosphate, nitrate and microorganism. Water quality standards, Analytical methods for measuring BOD, DO, COD, F, Oils, Metals (As, Cd, Cr, Hg, Pb, Se etc.). Residual chloride and chlorine demand. Purification and treatment water.

#### **Unit-III Atmosphere**

Chemical composition of atmosphere-particles, ions and radical and their formation. Chemical and photochemical reactions in atmosphere, smog formation, oxides of N, C, S, O and their effect, pollution by chemicals, petroleum, minerals, chlorofluorocarbons (CFC's). Greenhouse effect, acid rain, air pollution controls and their chemistry. Analytical methods for measuring air pollutants. Continuous monitoring instruments.

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# Unit- IV Green Chemistry: Definition and Objective

The twelve principles of Green Chemistry, atom economy in chemical synthesis, important technique employed in practice of Green Chemistry, Application of microwave irradiation and ultrasound in chemical reactions. Use of renewable raw materials and biosynthesis, organic waste management, use of safer reagents and green solvents and green catalysts.

# Unit-V Green Chemistry: Real Applications

Replacement of CFC and hydrocarbon blowing agents with environmental friendly blowing agent CO<sub>2</sub> in the production of polystyrene. Replacement of Ozone depleating and Smog producing solvents by surfactant assisted liquid or supercritical carbon dioxide for cleaning in manufacture of ICs and Computer chips.

#### **Books Suggested**

- Environmental Chemistry and Green Chemistry, Asin Kr Das, Books and Allied
   (P) Ltd. Kolkata.
- 2. Environmental Chemistry, H. Kaur, Pragati Prakashan.
- 3. Environmental Chemistry, S.F. Manahan, Lewis Publishers
- 4. Environmental Chemistry, A.K. Dey, Wiley Easlem.
- 5. Environmental Chemistry, C. Baird, W.H. Freeman.

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#### Semester- III

#### Core Course- XIII

#### **Bio-organic Chemistry**

Full Marks - 70

Credits-5

Unit- I

#### **Enzymes**

Basic considerations, Proximity effects and Molecular adaption. Introduction and historical perspective, chemical and biological catalysis, remarkable properties of enzymes like catalytic power, specificity and regulation. Nomenclature and classification. Concept and identification of active site by the use of inhibitors. Affinity labeling and enzyme modification by site-directed mutagenesis. Enzyme kinetics, Michaelis-Menten equation.

Unit- II

#### **Co-Enzyme Chemistry**

Cofactors as derived from vitamins, coenzymes, prosthetic groups, apoenzymes, Structure and biological functions of coenzyme A, thiamine pyrophosphate, pyridoxal phosphate, NAD, NADI, FMN, FAD, Lipoleic acid, vitamin B12, Mechanisms of reactions catalyzed by the above cofactors.

Unit- III

#### Carbohydrates:

Conformation of mono saccharides and important derivatives of mono saccharides, deoxycosides, deoxysugar, aminosugar, disaccharides, structure determination and chemical synthesis of sucrose, maltose and lactose.

#### Unit- IV.

#### Amino acids, peptides and proteinas:

Amino acids, essential and non essential amino acids, isoelectric point, amino acids sequencing primary, secondary structure,  $\alpha$ -helix,  $\beta$ -sheet structure of protein and tertiary and quaternary structures of protein

#### Unit- V.

#### Vitamins:

Classification, occurrence, Biological importance, structure determination and synthesis of vitamins A,B<sub>1</sub>,B<sub>2</sub> & C.

#### **Books Recommended:**

- 1. Understanding Enzymes- Trevor Palmer, Prentice Hall.
- 2. Enzyme Chemistry Impact and Application, Ed.- Collin J. Suckling, Chapma and Hail.
- 3. Enzyme Mechanisms Ed.- M.I Page and A. Villiams, Royal Society of Chemistry.
- 4. Fundamentals of Enzymology- N.C. Price and L. Slovens, Oxford University Press.
- 5. Immobilized Enzymes- An Introduction and Applications in Biotechnology, Michael O. Trevan, John Wiley.
- 6. Enzymatic Reaction Mechanisms- C. Walsh, W.H. Freeman.
- 7. Enzyme structure and Mechanism- A. Fersht, W.H. Freeman.
- 8. Chemistry of natural products –P.S Kalsi.
- 9. Natural products –Chemistry and Biological significance by J. Mann, R. S. Davison, J.B. Hobbs, Banthrope & J.B. Harborne.
- 10. Organic Chemistry- I.L. Phinar.

# Semester- III Core Course – XIV Practical (Inorganic Chemistry)

Full Marks - 50

Credits- 5

# Unit- I Either of the two from the following.

- 1. Quantitative analysis of two constituent ions of the following.
- (a) Cu, Zn (b) Fe, Ni (c) Ca, Mg (d) Al, Mg the cations

Mg<sup>++</sup> Ca<sup>++</sup> and Al<sup>+++</sup> can be estimated using EDTA.

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- 2. Green methods of preparation of the following and their study by IR, electronic spectra and T.G.A.
- (a) Pot trioxalato ferrate (III)
- (b) Pot trioxalato chromate (III)
- (c) Chromus Acetate
- (d) Hg[Co (SCN)<sub>4</sub>]
- (e) Hexa ammine Ni (II) chloride
- 3. Quantitative analysis of inorganic mixture containing six radicals including interfering radicals 15
- 4. Viva- voce
- 5. Note Book 5

#### **Books Recommended**

- 1. A text Book of Quantitative Inorganic Analysis A. I. Vogel
- 2. Applied Analytical chemistry- O.P. Vermani

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# Semester- IV Elective Course-1a Inorganic Chemistry Special

Full Marks - 70

Credits-5

# Unit- I (A) Alkyls and aryls transition metals.

Types, routes of synthesis, stability and decomposition pathways, Organocopper in organic synthesis.

# (B) 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 the ligands, Roles in organic synthesis.

# Unit- II Transition metal $\pi$ - complexes.

Transition metal  $\pi$  complexes with unsaturated organic molecules alkenes, alkynes, allyl, diene, dienyl, arene, trienyl complexes, their structural features and important nucleophilic and electrophilic reactions.

# Unit – III Homogeneous Catalysis.

Stoichiometric reactions for catalysis, homogeneous catalytic hydrogenation. Zeigler Natta polymerization of olefins, catalytic reactions involving CO, [e.g. hydrocarbonylation of olefins, (oxo reaction)], oxopalladation reactions, activation of C-H bond.

# Unit- IV (A) Application of Group Thery to CFF

d-orbitals as bassis of represention in octahedral field point derivation of Sine formula point use of Sine formula for splitting transformation of s,p,d,f,g,h orbitals in octahedral environment.

# (B) Application of Group Thery to

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Formation of Hybrid orbitals in tetrahedral, squareplaner, octahedral, square pyramid and TBP geometrics.

# Unit- V (A) Molecular rearrangement

D and A process, reactions of geometrical and optical isomers, optical inversions, isomerisation and recemisation of octahedral complexes, intermolecular rearrangement.

# (B) Fluxional organometallic compounds

Fluxionality and dynamic equalibria.

#### **Books Recommended:**

- 1. Organometallic Chemistry- Ayodhya Singh and Ratnesh Singh
- 2. Organometallic Chemistry- R.C. Mehrotra and A. Singh
- 3. The Organometallic Chemistry of transition metals- Robert H. Crabtree
- 4. Organometallic Compounds- Indrajeet Kumar.
- 5. Supramolecular chemistry- concept and perspective- J.M. Lehn
- 6. Introduction to Supramolecular chemistry- Helena- Dodziuk
- 7. Supramolecular chemistry Norendra N. Ghosh.
- 8. Photochemistry- Carle E. Wayne and Richard P. Wayne
- 9. Inorganic chemistry- Gary Walfsberg
- 10. Inorganic chemistry- J. E. Huhey, A. Keiler, L. Keiler, D.K. Medhi
- 11. Inorganic Chemistry G.L. Miessier and D.A. Tarr
- 12. Advanced Inorganic chemistry Cotton and Wilkinson T.

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# Semester- IV Elective Course- Ib Physical Chemistry Special

Full Marks-70

Credits-5

Unit- I (A) Hartree Fock Theory:

Born oppenheimer approximation. Salter-Condon rule, Hartree-Fock equation, Koopman theory.

(B) Semi Empirical Theories

HMO Theory of Conjugated dienes, D.E., Bond order, Free valence and charge density, and its calculation. Extended Huckel theory.

Unit- II Catalysis and Oscillatory Behaviour

Kinetics of catalytic reaction, Arrhenius intermediates, vant-Half intermediates, Theory of acid-base catalyst, Bronsted catalysis law, Hammet equation, Oscillatory reactions.

Unit- III (A) Kinetics of condensed phase Reaction.

Factors determining reaction rate in solution, Transition state theory in solution, kinetics of ionic reaction. Dependence of rate constant on ionic strength and dielectric constant of the medium. Bronsted Bjerrum equation.

(B) Study of Fast reactions.

Flash Photolysis, relaxation techniques, Molecular beam and shock Tube kinetics, stop flow method.

# Unit- IV Kinetics of Electrode reactions.

Faradic and non-faradic current rate law in faradic process, current density, factors affecting electrode-reaction, Effect of double layer structure on electrode reaction rates.

# Unit- V (A) Corrosion

Scope and economic of corrosion, causes and types of corrosion, electrochemical theories of corrosion.

# (B) Thermodynamics of solids

Specific heat of solids, Einstein and Debye theory of specific heat.

#### (C)Molecular Statistics

Thermodynamic probability, M.B., B.E. and F.D. statistics, comparision

#### **Books Suggested:**

1. Physical Chemistry : P.W. Atkins

2. Advance Physical Chemistry : Gurdeep Raj

3. Chemical Kinetics : Keith, J. Laidler.

4. An Introduction to chemical

thermodynamics : R.P. Rastogi & R.R. Mishra

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#### Semester- IV

#### **Elective Course-1c**

#### **Organic Chemistry Special**

Full Marks - 70

Credits-5

# Unit- I Terpennoids

Introduction, classification, isoprene rule and special isoprene rule. Structural determination, stereochemistry and synthesis of citral,  $\alpha$ -Terpeniol, camphor, santonin and abietic acid.

#### Unit- II Alkaloids

Introduction, classification, general method of structure determination. Structure and synthesis of the following compounds- Papaverine, Nicotine, Atropine, Quinine and Morphine.

# Unit- III Drug Design

Introduction, classification, SAR factors affecting bio activity. Theories of drug activity, Assay of drugs.

# Unit- IV Drugs

1. Antineoplastic Agents: Introduction, Cancer chemotherapy, role of alkylating agents, antimetabolites, natural products and hormones in treatement of cancer. Synthesis of mechlorethamine, cyclophosphamide, Fluoro-uracil, mustards, 6- mercaptopurine, melphalan.

- Cardiovascular Drugs: Cardiovascular disease, direct acting arteriolar dilators. Synthesis of amyl nitrate, sorbitrate, quinidine, Methyldopa, atenolol and oxyprenolol.
- 3. Anti-tubercular Drugs: PAS, Isoniazid, Ethambutol Thiosemicarbozone, Rifampicin.

# Unit- V Heterocyclic Compunds

- 1. Benzofused five membered heterocyclic compounds: Classification, nomenclature synthesis and reaction of benzopyrole, benzofuran and benzothiophenes.
- 2. Five and Six membered Heterocycles with two or more heteroatoms: Synthesis and reaction of oxazole, isooxazole, pyrazole, Imidazole, thiazole, diazine.
- 3. Seven and large membered Heterocycles with two or more heteroatoms: Synthesis and reaction of azepines, oxepines, diazepines. azocines and thiapines.

#### **Books Recommended:**

- 1. Natural Products-Chemistry and Biological Significance by J. Mann, R.S. Davidson, J.B. Hobbs, D.V. Banthrope and J.B. Harborne.
- 2 Organic Chemistry by I.L. Finar.
- 3 Rodds Chemistry of Carbon Compounds by S. Coffey.
- 4 Natural Products Chemistry by Jagdamba Singh and Jaya singh.
- 5 The Chemistry of Natural Products by P.S. Kalsi.
- 6 Chemistry of Natural Products by Nakamshi.
- 7 An Introduction to Medicinal Chemistry by Graham L. Patrick.
- 8 Textbook of Organic Medicinal and Pharmaceutical Chemistry by Charles O. Wilson, Ole Gisvold & Robert F. Doerge.

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- Principles of Medicinal Chemistry by William O. Foye, Thomas L. Lemice and David A. Williams.
- 10 Burgers Medicinal Chemistry and Drug Discovery by M.E. Wolff.
- 11 Heterocyclic Chemistry by R.R. Gupta, M. Kumar and V. Gupta.
- 12 Heterocyclic Chemistry by T.L. Gilchrist.
- 13 Organic Chemistry by I.L. Finar.

# Semester- IV Elective Course (P) 2 a **Practical (Inorganic Chemistry Special)**

Full Marks - 50

Credits-5

- 1. Qualitative analysis of Inorganic mixture containing six radicals including Mo, V, W, Ce 15
- 2. Analysis of atleast two metal ions in alloys and minerals
  - (a) Dolomite (b) Brass (c) Solder (d) Steel (e) Bouxite

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OR

Spectrophotometric determination of Fe, Ni, Mn, Cr, V, Ti, F, NO<sub>3</sub> and P04 etc.

Viva- Voce 3.

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4. Record File 5

#### **Books Recommended:**

- 1. Qualitative analysis- A.I. Vogel
- 2. Quantitative Analysis – A. I. Vogel

#### Semester- IV

# Elective course (P) 2b

# Practical (Physical Chemistry Special)

Full Marks- 50

Credits-5

Any one experiments (Marks 30)

- 1. Conductometric measurement;
  - (i) Dissociation constant of Acetic acid
  - (ii) Titration of Strong acid and strong base (NaOH+HCl)
  - (iii) solubility and Solubility Product of Sparingly soluble salts (PbSo<sub>4</sub>)
- 2. Potentiometric Experiments
  - Determination of (i) E.M.F. of Concentration Cell.
    - (ii) pH of a given solution using hydrogen electrode or quinhydrone electrode.
    - (iii) Acid-base titration.
- 3. Partition coefficients
  - (i) Determine the Partition coefficient of Acetic acid between Benzene and water.
  - (ii) Determine the partition coefficient of Iodine between CCl4 and water.
- 4. Viva-voce -15
- 5. Note Book -5

39