SYLLABUS

FOR

M.Sc. Chemistry

Semester (Ist, IInd ,IIIrd and IVth)

(CBCS- Based)

Effective from session 2018 -20 Onwards

University Department of Chemistry
B. R. Ambedkar Bihar University,
Muzaffarpur-842001

A.R.C 29/3/19

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

General Information:-

(1) It is two years Master Degree Programme

(2) There shall be four semester to complete programme. i.e. 1st,2nd, 3rd and 4thsemester

(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. Compulsory Courses, Core courses and Elective courses.

Core course –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 chosen from a pool of papers in IInd and IVthsemester.

(5) Each course will have 100 marks in full and divided as 70 marks for End-Semester Exam and 30 marks for Internal Assessment Work except in AEC, AECC-1, AECC-2 and practical papers. Internal assessment will be in two internal exams of 10 marks each, 5 marks for seminar/interhal project and 5 marks for attendance/discipline.

(6) In practical papers the distribution of marks in CIA will be same as prescribed forterm 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.

Credits- Aunit bywhich 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. 1st Semester

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

M. Sc. IInd Semester

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

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M. Sc. IIIrd Semester

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

M. Sc. IVth Semester

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

Candidates should choose 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**

? Bonding and Stereochemistry

Unit-I (a) VSEPR theory, Walsh diagram (triatomic molecules), dπ –pπ bonding, Bent rule and energetic of hybridization.

(b) M.O. diagram for hetero- nuclear di- and triatomic molecules.Bonding in Boranes, carboranes, Wades rule Anti ferromagnetic coupling.

Unit-II Magneto chemistry

e-e interaction, Term Symbols, spin orbit coupling Quenching of orbital contribution in metal complexes. Derivation of expression with small and large multiple width. Anomalous magnetic moments, magnetic properties of inner transition elements.

Unit-III Metal- Ligand Equilibria 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, chelate effect and its thermodynamic origin. Determination of formation constants by pH metery and spectrophotometry.

Unit-IV Reaction Mechanism of Transition metal complexes.

Inert and labile complexes, kinetic application of VBT and CFT, kinetics 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 planar complexes, The trans-effect, Theories of trans-effect, Electron transfer reactions-inner and outer sphere mechanism. Marcus-Hush theory.

Isopoly and Heteropolyacids.

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

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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
4. Introduction to ligand field- B.N. Figgis
5. Inorganic Reaction Mechanism- Basalo and Pearson
6. Chemical bonding- O.P. Agrawal/ Coulson
7. Structural Principles in Inorganic Chemistry-W.E. Addison
8. Introduction the Magneto Chemistry- A. Earshasw
9. Principle of Inorganic Chemistry- James Huhey.

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Semester-I
Core Course –II
Physical Chemistry-I

Full Marks -70 **Credits-5**

Unit-I **Macromolecules**

Types of polymers, Kinetics and mechanisms of polymerization, Molecular mass-number and mass average molecular mass, determination of molecular mass by osmometry, viscosity 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 limitation.
(iii) Quantitative treatment of Debye Huckle Limiting law and its modification for finite size ions, effect of ion solvent interaction on activity coefficients, Debye Huckle Onsager equation.
(iv) Butle-Volmer equation under equilibrium and non equilibrium Exchange current density, Tafel Plot.

Unit-III Chemical Dynamics

(a) Mechanism and Dynamics of consecutive and opposing reactions.
(b) Activated complex theory of Uni-molecular reaction.
(c) Mechanism and Dynamics of photolysis of acetaldehyde and photo dimerisation of Anthracene, Polymerization and Auto oxidation reaction. Study of fast reaction by flow method and relaxation method.

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, variation with 'T' and 'P', determination of Fugacity of a gas mixture, Duhem- Margules equation and its application.

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Unit-V **Statistical Thermodynamics**

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

Books Suggested: Recommended

1. Physical Chemistry : P.W. Atkins(ELBS)
2. Comprehensive Physical Chemistry : Hemant Snehil
3. Theoretical Physical Chemistry : Glastone.
4. Physical Chemistry : M.G. Barrow.
5. Modern Electrochemistry : JOM Bakris and A.K.N. Reddy
6. Text Book 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, tautomerism. Aromaticity in benzenoid and non- benzenoid compounds, alternant and non-alternant hydrocarbons, Huckel's rule, energy level of 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, prochirality, enantiotopic and diastereotopic atoms, groups and faces, asymmetric synthesis, 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. stability and reactivity of carbocations,

Unit-III **Reaction Mechanism: Structure and Reactivity:**

Types of reactions, kinetic and thermodynamic control, Hammond's postulate, Curtin-H ammet principle. Potential energy diagrams, transition states and intermediates, methods of determining mechanisms, isotope effects. Generation, structure,carbanions, free radicals, carbenes and nitrenes. Effect of structure on reactiviy. The Hammett equation and linear free energy relationship. substituent and reaction constants. Taft equation.

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Unit-IV **Aliphatic Nucleophilic Substitution:**

The SN^2, SN^1, mixed SN^1 and SN^2, SN^i and SET mechanisms. The neighbouring group mechanisms, neighbouring group participation by π and σ bonds anchimeric assistance. 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 $ArSN^1$,$ArSN^2$, 2Pso attack Benzyne and SRN^1 mechanisms. Reactivity-effect of substrate structure, leaving group and attacking nucleophile. The Von-Richter, Sommelet – Hauser, and Smiles rearrangements.

Unit-V **Aliphatic Electrophilic Substtitution:**

Bimolecular mechanisms – SE^2 and SE^1. Electrophilic substitution accompanied by double bone shifts. Effect of substrates, leaving group and the solvent polarity on the reactivity.

Elimination Reactions: Mechanism and orientation in pyrolytic elimination. Mechanism and application of Cope elimination, Chugaev reaction, Peterson reaction.

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Books Recommendation:

1. 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. Subdbrg.
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 **Duration of Exam 6 hrs.** **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 of inversion of cane sugar by using polarimeter.
7. i) Determination of Dissociation constant of acetic acid, by conductometric titration.
   ii) Solubility product of sparingly soluble salt.

Viva-voce-15

Note books-5

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Semester-I

AECC-1

Environmental Sustainability and Swachchha Bharat Abhiyan Activities

Semester-II
Core Course-V
Advances in Chemistry

Full Marks -70 **Credits-5**

Unit-I **Nuclear Chemistry**

(a) Shell model, Liquid drop Model, Nuclear Reactions and their Types. Nuclear Reactions Cross-section.

(b) Application of radio isotopes, tracer techniques, Neutron activation analysis, isotope dilution method.

Unit-II **Chemistry of Nanomaterials**

Definition, sources, examples, Bottom-up Method of synthesis, Characterizations, and applications

Unit-III **Solid state Chemistry**

Conductor, Semiconductor, and superconductor; Theory and Application

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.~~) ~~X. delete~~.

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Books recomended:

1- Industrial pollution: ~~by~~ Alka Gupta.
2- Solid State Chemistry: ~~by~~ Smart and Moore
3. Nuclear chemistry : Sharon and Sharon
4. Solid State Chemistry and its application : Anthony R West
5. The Chemistry of nanomaterials : CNR Rao, A. Muller & A. K. Cheetham.
6. Nanomaterials and their abbligation : Zihsan Hussain Khan Srivastava

Semester-II
Core Course-VI
Inorganic Chemistry II

Full Marks -70 **Credits-5**

Unit-I **Bonding in coordination Compounds:** Effect of distortion on d- orbital energy level. John- Teller effect,spectro chemical series. Thermo dynanic effect of crystal field Theory. Site selection in Normal and inverse spinal structure. Calculation of hydration energy and lattice energy of complexes. Evidences in support of covalent bonding in Transition metal complexes. M.O. Theory of ML_6 with σ and π -bonding liagands using symmetry arguments. Magnetic properties and charge transfer spectra on the basis of M.O. model.

Unit-II **Electronic Spectra of Transition Metal Complexes.**
Spectroscopic ground states, correlation and spin-orbit coupling in free ions for 1st series of transition metals, Orgel and Tanabe-Sugano diagrams for transition metal complexes (d^1-d^9 states), calculation of Dq, B and β parameters. Structural evidence from electronic spectrum, Spectrochemical and nephalauxetic series, charge transfer spectra, clectronic spectra of molecular addition compounds.

Unit-III **Symmetry in Chemistry.**
Symmetry elements and symmetry operations, definition of groups, sub-group, conjugate and class. Point symmetry group. Requirements of a mathematical group, multiplication table for C_{2v}, C_{3v}

Unit-IV **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-V **Metal π-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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Dinitrogen, tertiary phosphines as ligands. Metal Carbonyl clusters- Low Nuclear Carbonyl clusters Total electron count (TEC)

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 to quantum mechanics.

(i) Postulates of quantum mechanics, Angular momentum and Linear Operator

(ii) Hermitian operators, properties of operators.

(iii) Theorems of operators.

Unit-II Exactly soluble system.

(i) Linear Harmonic oscillator, Harmonic Vibration Hermite differential equation and its solution through recursion relation polynomial.

(ii) H-like atoms, separation or r,θ, φ equation. Laguerre and associated Laguerre Polynomial. Legendre polynomial equation and their solution.

Unit-III Approximate Method.

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

Unit-IV Huckel Molecular Orbital Theory.

Huckel theory of conjugated systems, bond order and charge density its calculation. Application to ethylene, butadiene, allyl and benzene

Unit-V Chemical Bonding

LCAO-MO theory, application of LCAO-MO theory to H_2^+ ion and H_2 molecule

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Recommended

Book Suggested:

1. Quantum chemistry : I.R. Lavine Prentiee Hall
2. Quantum chemistry : Pillar
3. Quantum chemistry : R.K. Prasad
4. Quantum chemistry : Satya PrakashSwati Saluja
5. Solid State Chemistry : D.K. Chakrabarty, New Age International
6. New Direction Solid State Chemistry : C.N.R. Rao & J. Gupal
7. Introduction to quantum Chemistry : A.K. Chandra, Tata

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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- and chemoselectivity, orientation and reactivity. Addition to cyclopropane ring. Hydroboration Michael reaction. Sharpless asymmetric epoxidation.

Free Radical Reactions

Allylic halogenations (NBS), oxidation of aldehydes to carboxylic acids auto-oxidation, coupling of alkynes, Free radical rearrangement Hunsdiecker reaction.

Unit-II **Photochemistry of carbonyl compounds.**

Photochemistry of enones, hydrogen abstraction. Rearrangements of α,β unsaturated ketones and cyclohexadienonies , photochemistry of p-benzoquiones.

Photochemistry of unsaturated system

Olefins, cis-trans isomerisation, dimerisation hydrogen abstraction and additions. Acetylenes-dimerisation, dienes-photochemistry of 1, 3-butadiene (2+2) additions leading to cage structures, photochemistry of cyclohexadienes, photochemistry of aromatic compounds-exited state of benzene and its 1,2 and 1,3-shifts, Photo-Fries rearrangement, Photo-Fries reacton 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 ally1 system, Classification of pericyclic reactions, Woodward-Hoffmann correlation diagrams, FMO and PMO approach, Electrocyclic reactions-conrotatory and disrotatory motions, 4n, $\overset{\pi}{4}+\overset{\pi}{2}$ and allyl systems. Cycloadditions-antrafacial and suprafacial additions, 4n and 4n+2 systems, 2+2 addition of ketenes, 1,3-dipolar cycloadditions and cheleoptropic rections.

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Sigmatropic rearrangement

Suprafacial and antarafacial shift of H, sigmatropic shifts involving carbon moieties, retention and inversion of configuration, (3,3) and (5,5) sigmatropic rearrangements deatailed treatment of Claisen and Cope-rearrangements. Aza-Cope rearrangements. Introduction to Ene reactins. Simple problems on pericyclic reactions.

Unit-IV Carbohyrate

Conformation of monosaccharides and important derivatives of manosaccharide- glycosides, deoxysugar, aminosugar. Structure determination and chemical synthesis of sucrose, and maltose.

Unit-V Amino acids, peptides and proteins

Chemical and enzymatic hydrolysis of proteins, amino acid sequencing. Secondary structure of protein, force responsible for secondary structure of proein, α- helix, β-sheet. Super secondary structure, tertiary structure of proteins folding.

Books Recommended ;

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Semester-II

Core Course –IX

Practical (Organic Chemistry)

Full Marks-50 **Duration of Exam 6 hrs.** **Credits-5**

1. **Quantitative Analysis**

Separation and identification of organic compounds in binary mixtures by chemical tests and preparation of their derivatives. 15Marks

2. **Organic Synthesis via two steps preparation** 15 Marks
   a. β-Nitroaniline from acetanilide.
   b. β-Bromoaniline from acetanilide
   c. β-Anthranilic acid from phthalic anhydride.
   d. β-Bromoacetanilide from aniline.
   e. β-Nitroacetanilide from aniline.
   f. β-Aminoazo benzene 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-II
AEC-1

Semester –III

Core Course-X

Principles & Applications of Spectroscopy

Full Marks-70 **Credits-5**

Unit-I Rotational Spectroscopy

Quantization of rotational energy and interactions of radiation with rotators. Classification of rotators; rigid rotator and Non-rigid rotator linear, symmetric and asymmetric rotators, isotopic effect, stark effect, effect of nuclear spin, and electron spin on rotational spectra, Bond length calculations.

Unit-II (A) Vibrational Spectroscopy

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

Unit-III Photoelectron Spectroscopy

Basic principles of photoelectric effect, ionization process, Adiabatic and vertical ionization energy,PESOS(UV-PES) and PESIS (XPES or ESCA). Chemical shift in ESCA. Chemical information from ESCA. Instrument and Techniques of Photoelectron Spectroscopy. Atomic electron spectrs of inert gases. Comparison of Photo-electron spectra of Ar, Kr, Xe. Photo-electron spectra of H_2 , O_2, N_2 and NO, HBr . XPES orESCA of Furan, Pyrrole and Thiophene. Zero kinetic energy , Photoelectron Spectroscopy, Auger Spectroscopy(AES), Scanning Auger Microprobes(SAM). Microscopic Technique : SEM, TEM, STEM,Focus ion beam Spectroscopy(FIB). Electron Microscope Koopman's theorem.

Unit-IV Magnetic Resonance Spectroscopy

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

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Nuclear quadrupole resonance spectroscopy. Basic Concepts of NQR., Electric field gradient, NQR frequency for N^{14} (I=1) B^{11}(I =3/2), ^{27}AL(I= 5/2) , .Nuclear quadrupole coupling constant.

Unit-V Applications of Spectroscopy

(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) Vibrational Spectroscopy

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_2, AB_3, AB_4, and AB_5. Hydrogen bonding.

(C) 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 ^{19}F and ^{31}P spectra of inorganic compounds.

(D) Mass Spectrometry Ion production and Fragmentation, molecular ion peak, Metastable peak, Mc. Lafferty rearrangement. Examples of mass spectra of organic compounds.

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Book ~~Suggested~~ Recommended:

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 pounds 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. Na^+/K^+ Pump, Role of metal ions 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, interaction between orally administered drugs and metal ions in gut.

Unit-II **Bioenergetics and ATP Cycle**

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

Unit-III **Transport and Storage of Dioxygen**

Heme proteins and oxygen uptake, structure and function of haemoglobin, myoglobin, hemocyanics and hemerythirn, 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 nitogenase, spectroscopic and other evidence, other nitrogenases model system.

Unit-V **Metals in Enzyme and Medicine**

The biochemistry of zinc, cobalt, nickel and molybdenum: Transport of Zinc, canbonic anhydrase, carboxypeptidase, alcohol dehydrogenase.,Adenosyl cobalamine as a coenzyme. Ribonucleotide reductase ,Methylcobalamine and cyano cobalamine as a co-factor, Nickel in urease, Hydrogenase, Molybdenum hydroxylase, Xanthine oxidase, Sulphite oxidase, nitrate reductase.

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Biochemical basis of essential metal deficient diseases., Iron copper and Zinc defficiency and their therapies, Carcinogens and carcinostatic agent, Zinc in tumors growth and inhibitial anticancer activeity and Mechanism of platinum, Rhodium, copper and Gold 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, Pd, Se, etc.). Residual chloride and chlorine demand. Purification and treatment of waste 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 effects, 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.

Unit-IV Green Chemistry: Definition and Objective

The twelve principles of Green Chemistry, atom economy in chemical synthesis, important techniques 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 green solvents and green catalysts.

Unit-IV Green Chemistry: Real Applications

Replacement of CFC and hydrocarbon blowing agents with environmental friendly blowing agent CO_2 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

1. 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 extraction and purification. Fischer's lock and key and Koshtand'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 Lineweave- Burk plots. Reversible and irreversible Inhibition.

Unit-II 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 chymotrypsin, lysozyme and carboxypeptidase A.

Unit-III Reactions Catalysed by Enzymes

Nucleophilic displacement on phosphorus atom, multiple displacement reactions and the coupling of ATP cleavage to endergonic processes. Transfer of sulphate, addition and elimination reaction. Enolic intermediates in isomerization reactions. P-cleavage and condensation, some isomerization and rearrangement reactions. Enzyme catalyzed carboxylation and decarboxylation.

Unit-IV 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,

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FAD, Lipole acid, vitamin B12, Mechanisms of reactions catalyzed by the above cofactors.

Unit-V Bioenergetics and Protein Metabolism

Free energy and entropy change in biochemical reactions. Synthesis of ATP. ATP as biological currency. Calvin cycle kerb cycle, glycolysis and glycogenesis. Amino acid metabolism, urea cycle. Chemical basis of heredity. Replication of DNA. Translation and Transcription.

Books Recommend:

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.

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

Full Marks-50 **Duration of Exam 6 hrs.** **Credits-5**

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^{2+} Ca^{2+} and Al^{3+} ~~can be estimated~~ using EDTA. 15
2. Green methods of preparation of the following complexes and their study by IR, electronic spectra and T.G.A. 15
   (a) Pot trioxalato ferrate (III)
   (b) Pot trioxalato chromate(III)
   (c) Chromus Acetate
   (d) $Hg[Co(SCN)_4]$
   (e) Hexa ammine Ni (II) chloride
3. Qualitative analysis of inorganic mixture containing six radicals including interfering radicals 15
4. Viva-voce 15
5. Note Book 5

Books Recommend:

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

Semester-III
AECC-2
Human values and professional ethics & gender sensitization

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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. Fluxional organometallic compounds, Fluxionality and dynamic equilibriai

Unit-II Transition metal π- complexes.

Transition metal π complexes with unsaturated organic molecules alkenes. alkynes, allyl, diene, dienyl, arene trienyl complexes, their structural features and important nucleophilic and elecrophilic reactions.

Unit-III Homogeneous Catalysis.

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

Unit-IV (A)SupramolecularChemistry

Introduction, Non covalent interactions, self-assembly in supromolecular chemistry, Reactivity and catalysis design and synthesis, transport processes and carrier design., superamolelcular devices.

(B) Photo chemistry of metal complexes.

Basis of photochemistry, properties of excited states, excited states of metal complexes and their comparison with organic compounds.

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Photo- substitution, photo-oxidation and photo-reduction, Excited electron transfer, Reactions of 2, 2-bipyridines and 1, 10 phenanthroline complexes, metal complexes sensitizers, Application of photochemical reactions of co- ordinance compounds.

Unit-V **(A) Molecular rearrangement**

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

(B) Spectroscopic Application: Application of Mossbauer and ESR spectroscopy in elucidation of structure of inorganic molecule.

Books Recommend:

1. Organometallic Chemistry- Ayodhya Singh and Ratnesh Singh
2. Organometallie Chemisty- RC.Mehrotr and A. Singh
3. The Organometailic Chemistry of transition metals- Robert H. Crabtree
4. Organometallic Compounds- Indrajeet Kumar.
5. Supramolecular chemistry- concept and perspective- J.M. Lehn
6. Introduetion to Supramolecular chemistry- Hiclena- Dodziuk
7. Supramolecular chemistry Norendra N. Ghosh.
8. Photochemistry- Carle E. Wayne and Richard P. Wayne
9. Inorganic chemistry- Gary Walfsberg
10. Inorganic ehemistry- J. E. Hulhey, 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-1b
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 π systems. Bond order, Free valence and charge density, and its calculation. Extended Huckle 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.

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Unit-V (A) Corrosion

Scope and economic of corrosion, causes and types of corrosion, electrochemical theories of corrosion, Method of protecting the corrosion

(B) Thermodynamics of solids

Specific heat of solids, Einstein heat capacity equation Debye theory of specific heat.

Books Suggested.

1. Physical chemistry	:	P.W. Atkins
2. Advance Physical chemistry	:	Gurdeep Raj
3. Chemical Kinetics	:	Keith, J. Laidler.
4. 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, α-Terpeniol, camphor, santonin

Unit-II Alkaloids

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

Unit-III Drug Design

(a) Introduction, classification of drugs. Development of new drugs. Procedures followed in drug design. Structure activity relationship. Receptor. Theories of drug activity with emphasis on Drug-receptors interactions.

(b) Application of Mass, IR, UV-Visible, NMR (^{1}H & ^{13}C) in elucidation of structure of organic molecules.

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, uracil-mustards, 6- mercaptopurine, melphalan.
2. **Cardiovascular Drugs:** Cardiovascular disease, drug inhibition of peripheral sympathetic function, direct acting arteriolar dilators. Synthesis of amyl nitrate, hydrolaxine verapamil, diazoxide propanol, sorbitrate, quinidine, Methyldopa, atenolol and oxyprenolol.
3. **Anti-tubercular Drugs:** PAS, Isoniazid, Ethambutol Thiosemicarbozone, Rifampcin.

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Unit-V Heterocyclic Compounds

1. **Benzfused five membered heterocyclic compounds:** Classification, nomenclature of aromatic heteroatoms: Synthesis and reaction of benzopyrole, benzofuran, benzothiophene.

2. **Five and Six membered Heterocycles1 with two or more heteroatoms:** Synthesis and reaction of oxazole, isooxazole, pyrazole, Imidazole, thiazole, diazine and tetrazines.
3. **Seven and large membered Heterocycles with two or more heteroatoms:** Synthesis and reaction of azepines, oxepines, diazepines. azocines and thiapines.

Books Recommend:

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 J.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 Organie Medicinal and armaceutical Chemistry by Charles O. Wilson, Ole Gisvold& Robert F. Doerge.
9. Prineiples of Medicinal Chemistry by Wilam 0. Foye, Thomas L. Lemice and David A. Williams.
10. Burgers Medicinal Chemistry and Drug Discovery by M.E. Wolft
11. Hetcrocylie Chemistry by RR. Gupta, M. Kumar and V.Gupta.
12. Heteroeyclic Chemistry by T.L. Gilchrist.
13. Organic Chemistry by I.L. Finar.

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Semester-IV

Elective Course (P) 2a

Practical (Inorganic Chemistry Special)

Full Marks – 50 **Duration of Exam 12 hrs.** **Credit – 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) Bauxite 15

OR

Spectrophotometric determination of Fe, Ni, M_n, Cr, V, Ti, F^-, NO_3^-, and PO_4^{---} etc,

3. Viva- Voce 15
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 **Duration of Exam 12 hrs.** **Credits- 5**

(Marks 30)

Two experiments have to be set.

1. Couductometric titration of strong acid and strong base (NaOH+HCl)
2. Potentiometrically pH of a given solution using hydrogen electrode or quinhydrone electrode.
3. Potentiometric Experiments Determination of Acid-base titration.
4. Determination of partition coefficient of Iodine between CCl_4 and water.
5. Determination of partition coefficient of $KI+I_2 = KI_3$ between CCl_4 and water.
6. Viva- voce -15
7. Note Book -5

Semester – IV
Elective Course (P) 2C
Practical Organic chemistry (Special)

Full Marks – 50 **Duration of Exam 12 hrs.** **Credits – 5**

Any two experiments have to be set (Marks 30)

1. Separation and identification of organic compounds using chemical methods from organic mixtures containing up to three components

2. Preparation of organic compounds involving several stages

3. Estimation of carbohydrates, protein, aminoacids, ascorbic acid, blood cholesterol and aspirin by UV – visible Spectrophtometric method.

4. Vivo Voce — 15 Marks
5. Note Book — 05 Marks

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Semester – IV
DSE-1

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Semester – IV
GE-1

A.R.E.
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