UNIVERSITY DEPARTMENT OF CHEMISTRY

RADHA GOVIND UNIVERSITY

RAMGARH, JHARKHAND

COURSE CURRICULUM FOR UNDERGRADUATE COURSES UNDER

CHOICE BASED CREDIT SYSTEM

M.Sc. (Honours in Chemistry)

With effect from 2018-2020

UNIVERSITY DEPARTMENT OF CHEMISTRY
RADHA GOVIND UNIVERSITY
RAMGARH

Semester – I			Course Credits	Hours /Week	Full Marks	End Sem + Mid Sem
S.	**Course**	**Course-Name**				
1.	CHE F-01 (Paper 1)	Fundamental of chemistry	5	5	100	70+30
2.	CHE C-02	Inorganic chemistry	5	5	100	70+30
3.	CHE C-03	Organic chemistry	5	5	100	70+30
4.	CHE C/P-04	practical	5	5	100	70+30
Semester – II			**Course Credits**	**Hours /Week**	**Full Marks**	**End Sem + Mid Sem**
S.	**Course**	**Course-Name**				
1.	CHE S-05	Skill development	5	5	100	70+30
2.	CHE C-06	Physical chemistry	5	5	100	70+30
3.	CHE C-07	Theoretical chemistry	5	5	100	70+30
4.	CHE C/P-08	practical	5	5	100	70+30
Semester – III			**Course Credits**	**Hours /Week**	**Full Marks**	**End Sem + Mid Sem**
S.	**Course**	**Course-Name**				
1.	CHE A-09(A/B/C)	Choice based elective	5	5	100	70+30
2.	CHE C-10	Inorganic chemistry	5	5	100	70+30
3.	CHE C-11	Organic chemistry	5	5	100	70+30
4.	CHE C/P-12	practical	5	5	100	70+30
Semester – IV			**Course Credits**	**Hours /Week**	**Full Marks**	**End Sem + Mid Sem**
S.	**Course**	**Course-Name**				
1.	CHE E-13(A/B/C)	Elective 1	5	5	100	70+30
2.	CHE E-14(A/B/C)	Elective II	5	5	100	70+30
3.	CHE E/P-15(A/B/C)	Laboratory course	5	5	100	70+30
4.	CHE D-16	Project/Dissertation	5	5	100	50+50

Regulation:

Each Paper (Theory & Practical) carries full marks of 100, out of which Sessional exam (Internals) will carry 30 marks and End Semester Exam (External) will carry 70 marks.

Sessional (Internals) Exam: 20 marks and General awareness, Attendance 05 and assignment 05.

End Semester Exam: 70 marks. The end semester exam will consist total nine questions. Candidates will be required to answer any five questions from long answer type questions. All questions will carry equal marks. Duration of paper will be of 3 hours.

M.Sc.
Chemistry
Semester-I
Fundamentals of Chemistry

Paper-I **CHEF-01**
Full Marks:70 **Time:3 hrs.**

UNIT-1 Mathematics for Chemists

A. Matrix

Matrix and determinant, The operation of Matrix algebra- Addition, subtraction and Scalar multiplication, Multiplication of determinants (of third order). Diagonal Matrix, Scalar matrix, unit matrix, singular and Non- singular Matrix, Transpose matrix, Adjoint matrix Orthogonal matrix and its properties. Inverse of a Matrix, Solution of Homogeneous and Non-homogeneous linear equations.

B. Vector

Introduction to Vector, Addition and subtraction of two vectors, Dot and cross products of two vectors, unit vectors, scalar and Vector products of unit vector, The gradient, Divergence and court.

C. Calculus

Differential calculus: Rules of Differentiation, Exact and inexact differential with their applications to Thermodynamic properties, Maxima and Minima (Examples related to Bohr radius and most probable velocity form Maxwell's distribution etc).

Integral Calculus: Basic rules for integration-Integration by parts, Partial fraction and substitution. Definite integrals and their evaluations.

UNIT-2 Operators:

Linear and non-linear operators, Hamiltonian operator, Hermitian operator and its significance, operators and commutation relations, Angular momentum operators and their commutation relations, operator using ladder operators.

UNIT-3 (a) Electronic structure of free atoms/ions-L-S coupling & J-J coupling Schemes, Determination of term symbols of p^n and d^n (n=1,2,3) systems, Hund's rule for deciding relative energies of terms, Selection rules for electronic transitions.

UNIT-3(b) VSPER theory-shapes of inorganic molecules/ions, Bent's rule and energetic of hybridization, Role of p and d orbitals in bonding and their implications, Simple reactions of covalently bonded moleucules.

UNIT-3 (c) Hard and soft acids and base, Classifications of acids and bases into hard and soft categories, Acid-Base strength and hardness and softness. Symbiosis, Theoretical basis of hardness and softness, Electronegativity and hardness and softness.

UNIT-4: Symmetry elements, Symmetry operations, Point groups, Systematic approach to determine the point group of molecules/ions, Multiplication of symmetry operations, Multiplication table for C_{2v},C_{2h} and C_{3v} Point groups (C_{2h} and -

C_{3v}), Use of character table in vibrational spectroscopy, Point group symmetry in the determination of dipole moment and optical activity of molecules.

UNIT-5(a) REACTION INTERMEDIATES

Generation, structure, stability and reactivity of Carbocations, Carbanions, Free radicals, Carbenes, Nitrenes and Benzynes. Application of NMR in detection of carbocations.

UNIT-5(b) REACTION MECHANISM: STRUCTURE AND REACTIVITY

Types of mechanism, types of reactions Thermodynamic and kinetic requirements, kinetics thermodynamic control, Hammond's postulate. Curtin-Hammett principle, Potential energy diagram, transition states and intermediates, methods determining mechanism, isotopic effects, Hard Soft acid and bases. Effect of structure reactivity – resonance and field effects, ste--- effect, Hammett equation and linear free energy relationship, substitution and reaction constants.

UNIT-5(c) NATURE OF BONDING IN OTGANIC MOLECULES

Delocalised chemical bonding –conjugation, cross conjugation resonance, hyperconjugation, bonding in fullerenes, tautomerism. Aromaticity in benzenoid and non-benzenoid compounds, alternant and non-alternant hydrocarbons. Huckel's rule, Energy level of molecular orbitals, annulenes, antiaromaticity, aromaticity, homoaromaticity.

M.Sc.
Chemistry
Semester-I
Inorganic Chemistry

Paper-II **CHEC-02**
Full Marks:70 **Time:3 hrs.**

UNIT-1

Pont symmetry group Schonflies Symbols, representations of groups by matrices (representation for the Cn, Cnv, Cnh. Dnh etc. groups to be worked out explicitly). Character of a representation. The great orthogonality theorem (without proof) and its importance. Character tables and their use; spectroscopy.

UNIT-2 STEREOCHEMISTRY AND BONDING IN MAIN GROUP COMPOUNDS **10 Hrs**

VSEPR, Walsh diagrams (tri- atomic molecules of type AH_2), dp pp bonds, Bent rule and energetic of hybridization, some simple reactions of covalently bonded molecules, Atomic Inversion, Betty Pseudorotation.

UNIT-3(a) METAL-LIGAND EQUILIBRIA IN SOLUTION **08 Hrs**

Limitation of crystal field theory, molecular orbital theory, octahedral, tetrahedral and square planar complexes, p-bonding and molecular orbital theory.

UNIT-3(b) METAL-LIGAND BONDING

Step wise 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 binary formation constants by pH-metry and spectrophotometer.

UNIT-4(a) METAL IONS IN BIOLOGICAL SYSTEMS **03 Hrs**

Essential and trace
metals.
Na^+/K^+ Pump
Role of metals ions in biological processes,

UNIT-4(b) BIOENERGETICS AND ATP CYCLE **04 Hrs**

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

UNIT-5(a) TRANSPORT AND STORAGE OF DIOXYGEN **05 Hrs**

Heme proteins and oxygen uptake, structure and function of hemoglobin, myoglobin, hemocyanins and hemerythrin, model synthetic complexes of iron, cobalt and copper.

UNIT-5(b) ELECTRON TRANSFER IN BIOLOGY **05 Hrs**

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 nitrogenases model systems.

M.Sc.
Chemistry
Semester-I
Organic Chemistry

Paper-III **CHEC-03**
Full Marks:70 **Time:3 hrs.**

UNIT-1 : STEREOCHEMISTRY OF ORGANIC COMPOUNDS

Optical isomerism: Fischer, Newman Sawhorse and Flying – Wedge projections and their introconversions, molecular symmetry and point groups, asymmetry and dissymmetry, stereochemical, descritors, centre of chirality, assigning of absolute stereochemistry, CLP rules, isotopic asymmetry, variation of specific rotation in sign and magnitude under different conditions, optical isomerism of compounds containing more than one asymmetric carbon atoms, number of stereoisomers, prochirality-topacity- homotopic and heterotopic, prostereoisomerism.

Geometrical isomerism: Nomenclature of geometrical isomers (E-Z notation) of compounds with one and more double bonds in acyclic system, methods of determination of the configuration of geometrical isomers in acyclic and cyclic system, interconversion of geometrical isomers.

Stereochemistry of aldoximes and ketoximes- naming, types of isomerism, methods of determining configurations.

Annulenes- Binary number methods of designing the sterecochemistry of annulenes.

UNIT-2: ELECTROPHILIC SUBSTITUTION REACTIONS

(a) Aliphatic electrophilic substitution: Bimolecular mechanism S_Ei, S_Ei and S_Ei mechanism Electrophilic substitution accompanied by double –bond shifts. Effect of substrates, leaving group and the solvent polarity on the reactivity.

(b) Aromatic electrophilic substitution: The arenium ion mechanism, orientation and reactivity, energy profile diagrams, The ortho para ratio, ipso attack, orientation in other ring system. Quantitative treatment of reactivity in substrates and electrophiles, Doazonium coupling , Gattermann Koch reaction, Vilsmeir reaction.

UNIT-3: NUCLEOPHILIC SUBSTITUTION REACTIONS

(a) Aliphatic nucleophilic substitution: The SN^2, SN^1, mixed SN^1 and SN^2 mechanisms. The neighbouring group mechanism, neighbouring group participation by Ω and π bonds.

(b) The SN^1 mechanism Nucleophilic substitution at an allylic aliphatic trigonal and at vinylic carbon. Reactivity effect of substrate structure, attacking nucleophile, leaving group and reaction medium, ambident nucleophile, regioselectivity.

(c) Aromatic Nucleophilic Substituion: The SN^{Ar}, SN^1, benzyne and S_{RN}^1 mechanism. Reactivity effect of substrate structure. Leaving group and attacking nucleophile. The vor Richter and Smiles rearrangement.

UNIT-4 (a) ADDITION TO CARBON- CARBON MULTIPLE BONDS

Mechanism and stereochemical aspects of addition reactions involving electrophiles, Nucleophiles and Free radicals, region and chemoselectivity, Orientation and reactivity, Addition to cyclopropane ring. Hydrogenation of double and triple bonds. Hydrogenation of Aromatic rings. Hydroboration, Michael reaction, Sharpless asymmetric epoxidation.

UNIT-4 (b) ADDITION TO CARBON-HETERO-MULTIPLE BONDS

Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acids, esters nitriles. Addition of Grignard's reagents, organozinc and organolithium reagents to carbonyl and unsaturated carbonyl compounds, Mechanism of condensation reactions involving enolates Aldol. Knoevenagel, Claisen, Mannich, Perkin and Stobbe reactions. Hydrolysis of ester and amides.

UNIT-5 (a) ELIMINATION REACTIONS

The E_2,E_1, and E_{1CB} mechanism and their spectrum, orientation of double bond. Reactivity- effects of substrate, Structures, attacking base, the leaving group and the medium.

UNIT-5 (b) MOLECULAR REARRANGEMENT REACTIONS

General mechanistic approach to molecular rearrangement reactions, Carbocation rearrangement, Migratory aptitutde and Memory effects, Brief study of following rearrangement reactions Pinacol-Pinacolone, Favoroskii, Baeyer-Villigers oxidations, Amdt- Eistert synthesis, Beckmann, Hofmann, Curtius, Fries and Claisen rearrangement.

BOOKS SUGGESTED:

1. Advanced Organic Chemistry – Reactions, Mechanism and Structure, Jerry March, John wiley.
2. Advanced Organic Chemistry – F.A Carey and R.J. Sundberg, plenum.
3. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman.
4. Structure and Mechanism in Organic Chemistry-C.S. Ingold, Cornell University Press.
5. Organic Chemistry- R.T. Morrison and R.N. Boyd, Prentice- Hall
6. Modern Organic Reactions- H.O., House, Benjamin.
7. Principles of Organic Synthesis – R.O.C. Norman and J.M. Coxon, Blackie Academic & Professional.
8. Reaction Mechanism in Organic Chemistry- S.M. Mukherji and S.P. Singh, Macmillan.
9. Stereo Chemistry of Organic Compounds- P.S. Kalsi, New Age International.
10. Stereochemistry of Organic Compounds – P.S. Kalsi, New Age International.
11. Advance organic chemistry, J. Singh and L.D.D. Yadav, Pragati Prakash, Meerut.

M.Sc.
Chemistry
Semester-I
Practical

Paper-IV **CHEP-04**
Full Marks:70 **Time:6 hrs.**

Two practicals are to be done selecting one each from two groups carrying 25 marks each have to be set in the examination

Group A

1. Quantitative Analysis — involving two of the following in Ores, Alloys or mixture in Solution, one by Volumetric and other by Gravimetric methods Ag, Cu, Fe, Cr, Mn, Ni, Zn, Ca, Mg, Cl and SO_4 .

2. Determination of COD and Hardness of water volulnetrically.
3. Preparation of selected Inorganic Complex compounds.

i) Cis — K $[Cr(C_2Od)_2(H_0)_2s$

ii) Na $[Cr(NH_3)_2(SCN)_4J$

iii) K; $[Fe(C_2Od)_3]$

iv) $[Ni(NH_3)_4]Cl_2$

v) $K_3[Cr(CtO_4)_3l$

Group B

4. **<u>Organic Synthesis</u>**

One Step organic Synthesis

(i) Benzophenone Oxiine from Benzophenone

(ii) Benzanilide from Benzophenone oxide (Beckmann Rearrangement)

”

(iii) Phthal imide from Plithalic anhydride

(iV) Anthanirlic Acid from Phthalimide (Hoffmann reaction)

(V) Ortho chloro benzoic acid from Anthranilic acid (Sandmeyer's reaction)

(vi) Bengil from Benzoin (Oxidation)

(vii) Dibenzyl from Benzil (Reduction)

(viii) Phenyl azo 9 — napathol from Aniline @iazo coupling)

(ix) 1-amino-2hydroxy naphthalene from Phenyl azo@ naphthol @eduction)

(x) Benzilic Acid from Benzil.

(xi) Fluorescein fom Phthalic anhydride.

(xii) m-nitro aniline from m-dinitro benzene (Reduction)

(xiii) Picric acid from phenol (niaation)

(xiv) Cinnamic acid from Benzaldehyde and malonic acid (Knovenagel reaction)

(XV) Dibenzal acetone from Benzaldehyde (Claisen Schmidt reaction)

(xvi) o acetanilide Aom Acetanilide.

Group C

1. Distribution Law

(a) To determine the partition coefficient of Benzoic acid or acetic acid between Benzene and water.

(b) To study the complex formation between Cu^{+2} and Ammonia and to determine the formula of the complex.

(c) To determine the equilibrium constant of the reaction $KI+I_2$ - KI_3

2. Chemical Kinetics

(a) To determine the velocity constant of hydrolysis of methyl acetate catalysed by HCl by ti4imeoic method.

(b) To determine the velocity constant of saponification of Ethy1 acetate conductomestrically

(c) To determine the acid catalysed reaction between I_2 and Acetone

3. <u>Viscosity</u>

(a) To determine the radius of molecules from viscosity measurement.

(b) To determine the composition of a liquid mixture

Viscometrically. Viva-voce 16 marks

Note Book 04 marks

Experiment 50 marks

Internal Assignment 20

marks Day to day internal Assignment

10

marks

Chemistry
M.Sc. Semester-II (Skill Development)

Paper-V (A) **CHES-05 (A)**
Full Marks:70 **Time:3 hrs.**

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

UNIT-1 Introduction to Computers and Computing
Basic structure and functioning of computers with a PC as an illustrative example, Memory, I/O devices. Secondary storage. Computer languages. Operating systems with DOS as an example. Introduction to UNIX and WINDOWS. Data Processing, principles of programming. Algorithms and flow-charts.

UNIT-2 Use of Computer Programmes
The students will learn how to operate a PC and how to run standard programmes and packages. Execution of linear regression, X-Y plot, numerical integration and differentiation as well as differential equation solution programmes. Monte Carlo and Molecular dynamics. Programmes with data preferably from physical chemistry laboratory. Packages- MS-Word, MS-Excel, FOXPRO, MATLAB.

UNIT 3: Potentionmetric analysis
Reversible cells, Types of cells, Liquid – Junction potential, Primary and secondary reference electrodes, measurement of E.M.F., Determination of (i) solubility and solubility product of sparingly soluble salts (ii) pH of a soluble salt. (iii) instability constant of a complex. Potentionmetric titrations.

UNIT-4: Spectrophotometric analysis
UV- visible, Lambert-Beer law, use of spectrophotometer in the determination of
(a) Percentage composition of a mixture.
(b) Ionisation constant of acid- base indicator
(c) Composition of complex (Job's method)

UNIT-5: Conductometric analysis
Conductance, Equivalent conductance, molar conducatance, Factor affecting different kinds of conductance of electrolytes. Principle of Vonductometric titrations,
Determination of
1. Dissociation constant of weak acid
2. Basicity of weak acid.
3. Hydrolysis constant of salt derived from a weak base and strong acid.
4. Velocity constant of saponification of ethy1 acetate.

Books Suggested

1. Comdex Computer Course kit (XP Edition), Vikas Gupta, Dreamtech, New Delhi
2. Fox Pro For DOS & Windows, R.K. Taxali, BPB Publication.
3. Programming in ANSIC, E. Balaguruswamy, Tata McGraw Hill
4. Compute for Chemist Bansal, Pragati Prakshan

M.Sc. Chemistry
Semester — II
S hill Development

Paper-V (B)

Time: 3 hr».

Full Marks:70

CHES-05 (B)

UNIT = 1 : ENVIRONMENTAL MONITERING

(a) Monitoring of water quality — Method of Sampling, Principle and prosedwe of the monitoring= BOD, COD, DO, Nitrite, Nitrate, Fluoride and Iron and Total E ardne.ss of water as in -vatcr samples.

(o) 7inalysis *Oi* Soil Samples - Principle and Procedure of tlne rni•.lysis of moisture, salinity, soil colJolds, cation and ai:ior. excl^.angc ‹:ap».city.

(c) Air pollution Monitoring — Sampling, Analysis of air pollutants such as S$ 2, NO , 3› .7 • nd suspended parties.late matter (SPM).

U7f I@ — 2 . PRINCIPLE OF ANALYSIS or roOD

(:i' Principle and procedure of Ai•.0lysis Of food « *epe'a'c!e pto‹ii.cis, Uill: aild pesticide residue.

(b) Pharmaceutical Analysis Principle & Procedure f Analysis of Aspii in, Vitamin A, Vitamin G, Vitamin Bi;.

(c) Clinical Analysis — Principle ‹?c .**iocedure of A.n lysis of Urea, f7rlticose, Albumin, Sodium and Potassium. (By Fla e Pliotometer Me od).

UNIT — 3 : ANALYSIS OF MET4LS & MINERALS

(a) .°iinciple and Procedure of the analysis or Brass, Ste :J, I..title stone, Ccrr.erit.

(b) Applicf.tion of i/V-Visible spectios'copy in qt al›ta'iv.: a›v1 quniititative analysis.

(c) Electro analytical technique Voltainetry, Polarograpliy, Conductometry & Chromatography.

(d) Coal — Ultimate and proximate analysis, bleating aalues -- grading of coals.

UNIT - 4: RISKS & HAZARDS OF CHEMICALS AND PROCEDURES

(a) Hazards of Handling ordinary chemicals, Fire hazards, Haiidling corrosive chemicals, Poisons chemicals.

(b) Cvcinogens Toxicity of Cd, Pb, Hg, As, Se, Pti, Oxides of Nitrogen & Sulphur, Benzen», £ialogenated hydrocarbons, Aromatic amino compounds, benzopyrine and related compound.s, Plastic Waste Management.

(c) Role of incineration in the production of carcinogens like dioxaiies Treatment of Hazardous waste and its disposal, ,Ra‹liocliemical wastes & technique of safe disposal of them.

UNIT – 5: FUNDA2dENTALS OF AGRICULTURAL Tt*›XIGOLOGY

T'oxicology, poison & poisoning, the. to::ivity of p•sticidos, ."!iresl'.o'id dose or T.L V. for some cominon clierr.ical toxic stib lethal dose, lethal dose, Toxicity indices (LD-50, EEi-50 etc.) Penetrati‹n of poisonous substances into cell-action on enzymes, Metabolism of poison in organism, Toxicity of pesticides to harmful organisms & factors determining it.

REFEREJCE§

l. Enviionmental c1iemis,try, S.E. M».iiah9n, Lewispublication.
2. Environmental chemistry, A.IC. De, Nevr /.gc, I:iten :itiona!.
3. Er:vironmenta1 pollutign Analysis,S.M. Khopkar, W ey Eastern.
4. Environmental ToSicology, Fid, J.Pose, Goidcn and Src.!.-i:, Sc:ence publication.

Chemistry
M.Sc. Semester-II
(Physical Chemistry)

Paper-VI **CHEC-06**
Full Marks:70 **Time:3 hrs.**

NIT 1: Ther modynamics

A. Classical Thermodynamics: Concept of free energy and entropy. Partial molar volume, Partial Molar entropy and Partial Nlolar free energy, Chemical potential. Effect of pressure and tempei”atUfC G:I Chemical potential, Determination of Partial molar‘ quantities by Graphical method and method of intercepts.

Fugacity, change of fugacity with te:nperatiire and pressize,’calcu!a!icn of fugac.ty (a) by graphical method (b) thorn Cainpi‘essibi1ity factor and (c) from equation of state.

B. Non- ideal systems: Activity ant1 activity co-effic ent, Debye Hiickel Theory for activity co-efficient of electroljtic solutions, determination of activity co-efficient, Ionic strength.

UNIT 2: Statistical Mechanics:

Stirling’s ".lpprocimation, Derivation of Bo1tzm.ann F9istribiltlOfi !*.s , partitio:i function and its Physics.1 significance, Re1atio1is’liip betv•eeli partition function and therinod"!Ia1TllC C,uantities e g. In e!nal energy, Entropy, Work function, Gibbs energy rnd Heat conta nt. Statistical

formulation of Third law of Thermodynamics, Derivation of relation between entropy and thermodynamics probability (S—k ln w) and Residual entropy.

Translational Partitifin function for a monoatomic Ideal gas, Entiopy and tran5lational Partition funciton (Sackur Tetrode equation), Partition Function for Rotational and Vibrational energy.

UNIT 3: Chemical Kinetics

Kinetics of Reversible First and ?>econd order reactions, kinetics of sequential l“irst order reaction and parallel reactions Derivation of .'Vrher.ius equation, Activation energy aitd its experiiv•.ntal :Ieterminations Frequency factor (A), Collision. theory ol reaction. x*.tss, far'.ure or collision theory, l’raiisition state I 1‹eor3',)iiiTet:t of !ei*.is :i?rength on !teaction rates -- Primary ai:c1 second:‹ry sa!t r.iTCCYS

The statiDnary State (steady state) liy;•.ot!i-.sis, Kinetics of Client:•. rerrctio-..s — Hydrogen — Bromine reaction, Decomposition of ethane aiid ellianal. Kinetics of Photochemical reactions — Hydrogen Chlorine and Hydrogen — Bromine reactions, oscillatory reactions — Belsusov — fihabati».s.-ii reaction (B Z reaction), Enzyme catalysts, kir.etics of enzyme catalyiis — lvhchaelis — Menten equation and Its irapor!ance

UNIT 4: Electorchemistry;

A. D4b-•e Hiickel limit,tng latv oi :ic:›.vity «o-efficient of ele°v›.•»l ‹ts., verification and limitations 8f Debye — Huc1:el theory anc its ext•nsioH to lnake allowance for finite size and ionic asscciatfcn pararileter

Measurement of activity co-efficient by solubility, freezing point depression and e.m.f methods, Effect of ion- solvent interaction on activity co-efficient of ions (Robinson stroke treatment). Overpotential, Exchange current density, Derivation of Butler-Volmer equation and Tafel plot.

Unit 5 (a) : Surface Chemistry

Derivation of Gibbs adsorption Equation, Surface film, Langmuir Theory of Adsorption. Derivation of the BET equation and Estimation of surface area. Thermodynamics & statistical Mechanics of Adsorption.

Chemical Reaction of Surface- Unimolecular reactions, Bimolecular reactions and Langmuir – Hinshelwood mechanism, Langmuir – Rideal mechanism.

Unit 5(b) : Laws of Photochemistry, Quantum yield, Reasons for high and low quantum yield Photolysis of HI and its kinetics, fluorescence, Phosphorescence, Chemical reactions and their quantum yields, Photosensitization, Photosynthesis, Photostationary state, Chemiluminescence and Thermoluminescence, Photography, Photochemical cells, The Carbon monoxide oxygen Reaction, Kinectics of collisional quenching – Stern- Volmer equation and deviation from stern- Volmer equation and deviation from stern- volmer equation, E-type P-type delayed fluorescence.

BOOK SUGGESTED:

1. Physical Chemistry — P.W. Atkins, ELBS.

2.. A. Text Book of Physical Chemistry — S. Glasstone, McMillan.

3. Physical Chemistry Alberty and Daniels.

4, Chemical kinetics — K.J. hardier, 1\Ie Grow Hill.

5. Modern Electro Chemistry Vol.-I & Vol.-II — JOM Bockris A AKN Reddy, Plenum.

6. Mathematics for Chemistry — Doggett and Sucliffe, Langman.

7. Basic Mathematics for Chemists Tebbt:9, ^Yile

8. Physical Chemistry A. lviolecular Approach Ei./ ,Ms Quarrie and J.D Simon; Viva Books Pvt. Lid.

Chemistry
M.Sc.
Semester-II
(Theoretical Chemistry)

Paper-VII **CHEC-07**
Full Marks:70 **Time:3 hrs.**

UNIT - 1 Quahtum M8thanical Results:

Solution and discussiqn of the Schrodinger equation to some model systems viz. Particle in three dimensional box, Particle gon a ring, The harmonic oscillatbr, The rigid rotor, . The hydrogen atérh, simple and generalised treatment.

UNIT - 2 Approximate iYtethods:

First order Anne indep ndent Per •zbation theory for non-d.eg•nerate states. The variation theor m, Application of variation iethoil ac:1 perturbation theory to he.lium atom.

UNI"f—3 **HucJel Mold ar orbital The ry**

HilkJl the:ry of cJ jugated syste is; 4ipplicatii n ’d HMO to Ethene. Rutadi$n , Cyclb openyl radical and cyclobiiiadi$ne. Bond order and charge ensity c lations.

UNIT — 4’ Microwave spectroscopy

Classification of molecules, Rotational energy levels, Isotope effect in Rotational specCa, Intensity of rotational .lines, Non-rigid rotator, vibrational Excitation!Effect, Symmekic Top molecules, A symmetric top molecules, stark effect, Information..derived ñom Rotational spec4a.

UNIT — 5(a) Infra-red spectroscopy

Vibrational Energy of a diatomic molecule, zeropoint energy, force constant, Anharmonicity, Morse potential energy diagram, Vibration — rotation spec4oscopy, P, Q, R Branches, Vibrations of poly atomic molecules, normal modes of. vibration, overtones, factors affecting the band positions and,intensity.

UNIT - 5(b) Raman Spectroscopy

Classical and quantum theories of Raman SpecYum,, ‘Rotational Raman Specoa Linear molecules, Syrnmeti’ic Top molecules,. Vibrational Raman Spec4a, Mti{ual Exclusion Principle.

BOOKS RECOMMENDED:

1. Modern specoooscopy, JNd Eoilas, Jolnl, Wiley.
2. Introduction to MolecJlar spcctroscopy, G.M. Barro w.
3. Molecular stmctwe & §pectroscopy, O. Aruldhas, P HI
4. Modern Molecular Sp “fioscopy, H S Randhawa M cmillan.
5. In4odiiction to Quanturn Chemistry; A..K. Chrndrq, lata Mebraw Hill.
6. Quanttun GhJemistry, Levine, PHI.

Chemistry
M.Sc.
Semester-II
(Practical)

Paper-VIII **CHEP-08**
Full Marks:70 **Time:6 hrs.**

Two practicals selecting one from each of the two groups carrying 25 marks each have to be set in the examination.

Group A

1. Qualitative Analysis of mixture containing 8 radicals including some less common metal ions anal interfering radicals from among the following by comlnon method (Preferably Seini Micro)

   Basic radicals

   Pb, Cu, Cd, Bi, Sn, Fe, Al, Cr, Zn, hIn, Co, Ni, $a, Sr, Ca, l?i;, Na, IN, NIJ

   Acid radicals

   Carbonate, Sulphate, Siilphite, Nitrite, Acetate, F1'ioride, Chloride, Bromide, Iodide, Nitrate, Borate, Oxa!ate, Pliospb...‘.e, Silicate, Chromate, Arsenite, Arsenate, Perinangaiiate.

Group B

2. Estimate of Glycine
3. Estimate •›f Glucose
4. Determination of saponification valu{ of given oil/ flat.
5. Estimation of Phenol
6. Estimation of Hydroxyl yoiiJi.
7. Determination of equiva!ent wt ‹if oarboxylic acid b$ Titre.‹io!l method.

8. Determination N-acetyl group in organic compound.

Group C

Conductometry

9. Determination of tlte velocity constant, order of reaction and of activation of Sapanifiv-atiOn of Ethyl acetate by NaOH conductometrically Energy

10. Determination of solubility and solulaility product of sparingly soluble salts. (e,g. PbSO4, BaSO, etc.) conductometrically.

11. To study the effect of solvent on the conductance of AgNO3 Acetic Acid and to det•rmine the depee of dissDciatioii :ll2d equilibrium constant in different solvents and in their mixture (DMSO, DMF, Dioxane, aceion», water) and to test the Validity of Debye – Onsager 'equation.

12. Determination of activit ʳ co•l'ficie:it ol' Zn" iit the soll!tio:i o/ 0.02 M, ZnSO, using Debye-Hltclcel Limiting law:

Potentiontetry / pH metry

13. Acid — Base titration' in a non--aqtieous medium us ng pH meter.

14. Determination of strength of sCoiig and v/ealx a id of a give:i mixture using potentionineter /pH meter.

Use of Abbe's Refractoizi ter

15. Determination of reftactive inde:i .«.nd molecular r fretivity of a liquid.

Vivz -â»ce	16 r.call:s
Note Book	04 i:iarlis
Experiment	50 inaiks
Interval Assignment	20 marks
Day to day interval Assignment	10 marks

M.Sc.
Chemistry
Semester-III
(Choice Based Elective)

Paper-IX (A) **CHE-A-09**

(A) Full Marks:70 Time:3 hrs.

METAL –LIGAND EQUILIBRIUM IN SOLUTION AND INORGANIC REACTION MECHANISM

UNIT 1 : Stability of complexes in aqueous solution

Stability of complexes, Stepwise and overall stability constants and their relationship, Kinetic versus thermodynamic stability, Trends in stepwise formation constants, Factors affecting stability of complexes, Chelate effect and its thermodynamic origin, Experimental methods for the determination of stability constant and composition of complexes by spectrophotometric method, Job's method & Bjerrum method.

UNIT 2 : Ligand substitution reactions in octahedral complexes

Reactivity of metal complexes, Inert and labile complexes, Valence bond and crystal field interpretation of lability and inertness of the complexes, Rate laws and their interpretation – The Eigen – Wilkins mechanism & Fuoss – Eigen equation, The activation of octahedral complexes, Mechanism of ligand substitution reactions in octahedral complexes, Hydrolysis reaction – acid hydrolysis (S_N1 mechanism), base hydrolysis (S_N1_{CB} mechanism) Evidences in farour of S_N1_{CB} mechanism.

UNIT 3 : Ligand substitution reactions

The trans effect, theories of trans effect, Difference between trans effect and trans influence, Trans effect series, Mechanism of ligand substitution reactions in square planar complexes, Factors affecting the rate ligand substitution reactions in square plannar complexes, Applications of trans effect.

UNIT 4 : **Electron transfer-reactions**

Basic concepts of oxidation and reduction, reactions, Electron transfer reactions in coordination compounds by outer sphere and inner sphere mechanisms, The marcus theory and the factors affecting the rate of electron transfer reactions by outer sphere mechanism, complementary and non-complementary electron transfer reactions.

UNIT 5 : **Photochemical reactions**

Basic concepts of photocheinistry, Photochemical and thermal excitation of complexes of complexes and fates of excited complexes, Photochemical reactions of cobalt (III) and chromium (III) complexes, photo-oxidation, Photo reduction, lntervalence transitions.

BOOKS RECOMMENDED

1. Elements of Inorganic Pliotoclieiriistry, W.J. Ferraudi, Wiley
2. Inorganic Chemistry, Shriver and Atklns, Oxford University, Press
3. Concepts of Inorganic Photocheinistry, A.W. Adamson *S* P.D. Fleiscliain, Wiley.
4. Selected Topics in Inorganic Chemistry, Madan, Mallk & Tuli, S. Cliand

M.Sc.
Chemistry
Semester-III
(Choice Based Elective)

Paper-IX (B) **CHE-A-09**

(B)Full
Marks:70
Time:3 hrs.

UNIT -1 Selectivity

Types of selectivity : Regio, Stereo and Chemoselectivity, Reagents for reduction of alkenes, alkyes, arenaes and carbonyl compounds, mechanism of action – dissolving metal reduction, Removal of functional groups, reduction of benzene rings and alkynes, Protection of aldehydes, ketones, alcohols and amines, carrying out reaction at less reactive group in the presence of more reactive group, Reagents for chemoselective oxidation of (a) C=C double bonds e.g. peracids, osmium tetraoxide, ozone etc. and (b) alcohols and carbonyl compounds e.g. Cr(VI) and Mn(VII) compounds. Peptide synthesis : The Cbz protection group and removal, t-Boc protection group and removal, and the Fmoc protection and removal – Merrifield approach.

Unit -2 Making new C-C bond

A) Alkylation of nitroalkanes, alkyl nitriles, Lithium enolates of carbonyl compounds such as ketones, esters, and carboxylic acids. Alkylation of aldehydes and ketones using specific enol equivalents such as enamines (Stork enamine reaction), silyl enol ethers, azaenolates derived from imines. Regioselective formation of enolates from ketones, thermodynamic enolates and kinetic enolates. alkylation of β-dicarbonyl compounds, Regioselective

reduction of enones; formation of enolates regiospecifically, conjugate addition to enones to give enolates regiospecifically

B) Acylation at Carbon

Directed C-acylation of enols and enolates, Acylation of enols under acidic conditions, acylation at nucleophilic carbon (other than enols and enolates)

C) Conjugate addition of enolates -

Conjugate addition (i) Under thermodynamic control (ii) Under kinetic control condition, Conjugate addition of (i) enols (ii) enolates (iii) enamines (iv) silyl enol ethers : Electrophilic alkenes exo-inethylene ketones a component obtained from Mannich reaction, nitroalkanes, Robinson's annealation reaction, Use of Lithium dimethyl cuprate.

D) Carbon bond formation using radicals, Tributyltinliydride, nucleophilic and electropliiclic radical, Comparison of reactivity pattern of radicals and polar reagents, Comparison between Intermolecular and Intra molecular radical reactions, Barlon and Hoffmann — Loffler — Freytzag reaction.

Unit -3 The Aldul reaction

Introduction, acid and base catalysed reactions, Aldol reaction of unsymmetrical ketones, crossed condensation Conditiones of successful crossed aldol reaction. Controlling aldol reactions witlt specific enol equivalents; use of following enolates in aldol reactions lithium eñolates, silylenolethers, zinc enolates, aza enolates, enamines; use of conjugated Witting reagents as specific enol equivalents in aldol reaction. Specific. enol equilvalent for (a) carboxylic acid derivatives, (b) free carboxylic acids, (c) aldehydes and (d) ketones preparation of (i) kinetic

and (ii) thermodynamic enolates. lntramolecular aldol reaction, Overview of equilibrium and directed aldol methods.

Unit -4 Creative Chemistry

Retrosyntliic analysis, Syntllons, classification of syntlioits, Different terminologies, Umpoltlng reactions, Disconnections Guidelines for good disconnections, Functional grotip interconversions, C-C disconnection, Two group C-C disconnection :- 1,3 difunctionalized compounds, 1,2 difunctional compounds, 1,4 difunctional coivtpounds.

Synthesis of (i) Penicillin (V) and Ceftazidime with emphasis on retrosynthetic anlysis. (ii) lbogamine — elnphasis on stereocontrol of the synthesis.

UNIT - 5

Synthesis using reagents containing Phosphorous, Stllfur or boron.

1. Pl+osphorous containing reagents:

Reactions of phosphorous ylides; Redtictive cyclization of nitro compounds; Synthesis of alkenes froin 1, 2 diOls, COilversiOn of alcohols into aldehydes.

2. Sulfur containing reagents:

Reactions of sulfur ylides, sulfoxide elimination, use of dithioacetals, reversed polarity of carbonyl coinpotlnds, Julia reaction.

3. Boron containing reagents:

Reactions of organoboranes from alkenes: Oxidation to alcohols, conversion into primary amines, carbonylation — synthesis of 2” and 3^0 alcohols, Ketones and aldehydes.

Cyanidation and synthesis of esters. Reactions of organoboranes from alkynes; Synthesis of ketones and aldehydes, synthesis of E and Z alkenes, Synthesis of conjugated dienes and synthesis of bromoalkenes.

Ref :

(1) Organic chemistry : Clayden, Greeves, Warren and Wothers Oxford university Press

(2) Organic Synthesis : R.O.C. Norman & Coxan

(3) Modern methods of organic synthesis W. Camither

M.Sc.
Chemistry
Semester-III
Choice Based
Elective

Paper-IX (C) **CHE-A-09**

(C)Full
Marks:70
Time:3 hrs.

UNIT 1 Band Theory & Electronic Properties

Band theory of solids, conductor, Insulator and Semi-conductor, Propagatlon of Broglie waves in solids, Brillouin Zones, Distribution of density of states.

Semi-conductors: Intrinsic semi-conductors, Number of e1ecti'ons in a ondu tion Band, Extrinsic Semi-conductor, The p-n junction, The p-n junction as a rectifier, super-conductors, Pliotoelectric Effect, Thermocouples, The Hall effect.

UNIT 2 Organic Solids

E ectrically conducting organic solids, organic metals — conjugated systems — Doped poly acetylene, Polyparaphenylene, poly pyrrole, organic charge transfer complexes — New Superconductors.

UNIT 3 Phase Transitions

Thermodynamic classification of Phase transitions, Applications of G — T dia am; Stable phases and inetastable phases, kinetics pf Phase transitions, critical size of nuclei, Rate equations — Nucleation Rate, overall transfom ation rate — Avramic equation, Factors that influence thg kinetics of Phase transitions, order — disorder transitions.

UNIT 4 Properties of Insulators

Electrical Properties — Dielectric Properties, polarisation density and elecaic suscepti/ility, Loren% force and field, Clausius Mosoni equation, piezoelectricity, Ferroeleckicity, Ionic conductivity and ionic difRsion, Elecoic breakdown,

Magntetic P roperties — Antiferromagnetism, and curie temperatwe, Ferrimagnetism and Magnetic Resonace.

UNIT 5 Crystal defecG and Reciprocal lattice

Crystal defects - Point, line and plane defects, schottky defect, frenkel defect, Thermodynamics of Schotly and frenkel defect formation, colour centres;

Reciprocal &ttice — Receprocd lamce and its properties, Bragg's equation in reciprocal lattice.

UNIT 6 Specific heat of solids

Einstein's theory of specific heat and its limitations, Debye's continuum model — Debye T^3 law. Deviation from the Debye theory.

Bodks Sugguted

1. Physical Chemistry — R.A. Alberts wiley Eastern Ltd.
2. Solid state chemistry and its applications — A.R. w› st wiley India Pvt. Ltd.
3. In4oduction to solids — Azaroff, TMH Edition.
4. Physical Chemistry, G.M. Barrow, TMH Edition.

M.Sc.
Chemistry
Semester-III
(Inorganic Chemistry)

Paper- X **CHEC-10 Full**

UNIT – 1: Chemistry of main group elements, Synthesis, properties and structure of Boranes, Carboranes, Borazines, Silicates, Silicones Phosphazenes and S-N ring & chain compounds.

UNIT – 2: Crystal field theory – splitting of d orbitals in low symmetry environments (square planer, square pyramidal & trigonal bipyramida fields), structural effects of orbital splitting, Jahn-Teller effect and its implications, thermodynamic effects, crystal field stabilization energies for octahedral and tetrahedral complexes, correlation of CFSE with related thermodynamic properties such as lattice energies, enthalpy of hydration, stabilization of unusual oxidation states, CFSE and structure of spinels.

UNIT – 3: Limitations of crystal field theory, evidences in favour of M-L orbital overlap – Nephelauxetic effect, Molecular orbital theory, Molecular orbital diagram of tetrahedral and octahedral complexes with and without π bonding, Studies of spectral properties transition metal complexes, splitting of terms of d^1 and d^2 ions in octahedral, tetrahedral and square planar fields, Orgel diagram, Tanabe-Sugano diagram, Racah parameters and their calculation.

UNIT – 4: Complexes with π acceptor ligands, Metal carbonyls-mononuclear, binuclear, trinuclear & ploynuclear carbonyls and their preparation, properties, structure, bonding & applications, Reactions of coordinated CO. Metal nitrosyls-preparation, reactions, bonding &

Marks:70
Time:3 hrs.

structure, Reactions of cooi dinated NO. Dinitrogeii and dioxygen complexes

UNIT — .5: Metal metal bonding aitd iitetal cluster compounds : M-M multiple bonds, Factors favouring the fiirinatioii of M-M bond, Evidences in support of M-M bond, Metal Clusters- classification-diittlclear clusters, trinuclear clusters, tetranuclear clusters & liexaitrlclear cltlstei's, Syntliesl S and important reactions of metal clusters

Book recommended

1. Advanced lilorganic Chemistry, Cotton and Wilkinson, Jolili Wiley & Sons.
2. Inorganic Clielnistry Principles of Sti ticttu e and Reactivity, Htllieey, Keiter & Keiter, Harper Collins Colleges Publishers.

3 Modern Inorganic Chemistry W.L. /o1ley, McGraw Hill

M.Sc.
Chemistry
Semester-III
(Organic Chemistry)

Paper-XI **CHEC-11 Full Marks:70**
Time:3 hrs.

UNIT — 1: PHOTOCHEMISTRY :

1. Basic concepts, Electronic transitions, JablonslAi diagram, Intersystem crossing, Energy transfer, Molecular orbital view of excitation.
2. Photochemistry of Alkenes : Intermolecular reactions of olefinic bond, geometrical isomerism, cyclisation reactions, rearrangement of (1,4) — and (1,5) — dienes, di - methane rearrangement.
3. Pliotochelnistry of Carbonvl : Compounds : Iner-molecular reactions of Carbonyl Compounds, saturated cyclic and acyclic, b, y unsaturated and o, b unsaturated compounds, cycloliexadienone Intermolecular cycloaddition reactions, Diinerisatlons and oxetane formation.
4. Photoclielnistrv of Aromatic compounds : Isomerisation, Additions, substitutions.
5. Miscellanceous Photochemical reactions : Photo Fries reactions of anilldes, Photo Fries rearrangement, Barton reaction, Slnglet molecular oxygen reactions, Photochemistry of vision.

UNIT — 2: PERICYCLIC REACTIONS :

Molecular orbital symmetry, Frontier orbital of ethylene, 1, 3 — butadiene, 1,3,5- hyexatriene and allyl system. Classification of Pericyclic reactions. Woodward — Hoffmann correlation diagrams, FMO and PMO approach. Electrocyclic reactions, Conrotatory motions, 4n, 4n+2 and allyl systems, (2+2) addition of ketenes, 1,3 dipolar cycloadditions and clielotropic

reactions. Sigmatropic rearrangement suprafacial and antrafacial shifts of H, sipnatropic shifts involving carbon moieties, (3,3) and (5,5) sigmatropic rearaangements. Claisen, Cope and aza-cope reaxrageinents. Fluxional tautamerism, Ene reaction.

UNIT — 3: SPECTROSCOPY — APPLICATIONS IN ORGANIC CHEMISTRY :

1. UV-VIS Spectroscopy : Electronic transitions of enes, enones and arenes. Woodward-Fieser rules. Effect of solvent polarity on UV absorption, Application of Woodwar-Fewser rule for calculating absorption maxima in cyclic and acyclic conjugated dicnes and enones. Problems based on the above rules. Carbonyl chromophores, Steric hindrance and coplanarity — distinction between cis and trans isomers.
2. II? Spectroscopy : Vibration-rotation spectrum Theory of molecular vibrations, stretching, bending vibrations. Hydrogen bond and ffeqiiency distinction between inter and intramolecttlar hydrogen bonding. Finger print region. Characteristic group frequencies of OH group in alcohols and phenols, CO group in aldehydes, ketones, acid chlorides, acid anhydrides, amides and esters. Simple problems based on these data.
3. NMR Spectroscopy : Chemical shift, anisotropic effect and coupling constants in organic compounds. Spin-spin interactions in typical 5yste1ns. Effect of magnetic field stren@h on sensitivity and resolution. Karplus relationship of I on diliedral angle. C^{13} chemical shifts. Spectral interpretation and structure identification. Solving of structural problems on the basic of numerical and spectrum based data.

4. Mass Spectroscopy : Fragmentation pattern, molecular ion peak, metastable peak, McLafferty rearrangement, Examples of mass spectral fragments of organic compounds Solving of Structural problems
5. Combined applications of UV-Visible, IR, NMR and Mass spectroscopy in structure determination of organic compounds.

REFERENCE:

1. W.Kemp, "Organic Spectroscopy", Longman.
2. Jerry March, "Advance Organic Chemistry"
3 Organic Spectroscopy by Y.R. Sharma
4 Introduction to Organic Spectroscopy, Silverstein
5. Fundamentals of Photochemistry by K.K. Rahtogi Mukliargee
6. Organic Chemistry by Cleyden, Oxford University Press
7. Ofgaiiic Reaction & Mechanism by Singh & Mukharjee
8. Pericyclic & Photochemistry – Yadav Singh
9. Spectroscopy – Kalsi, Pragati Prakasliae
10. Conservation of Orbital Symmetry – Woodward & Hoffman.

M.Sc.
Chemistry
Semester-III
(Practical)

Paper-XII **CHEP-12 Full Marks:70**
Time:06 hrs.

Two practical selecting one from two groups carrying 25 marks each have to be set in the examination.

Group A

1. Determination of standard deviation and correlation coefficient.
2. Plotting of graph by least square method.
3. Quantitative calculation based on Beer's law.
4. Analysis of Dolomite, Pyroliisite and Haematite.

Group B

5. Identification of organic compounds containing not inore than two functional groups, (Ten compounds are to be identified in the lab work.)

Group C

6. To determine the equivalent conductance of an electrolyte at infinite dilution and determine the dissociation constant.
7. To deterlnine the pKa of given dibasic and tribasic acids pH inetrically.
8. To determine the pH of various mixtures of acetic acid and Na-acetate in aqueous solutions and Jience the dissociation constant of the acid.
9. Titrate ferrous aminoniuin sulphate against $K_2Cr_2O_7$ /KMnO, and determine redox potential of Fe^{+2} / Fe^{3+} system potentioinetrically

10. To determine ionization constant of polybasic acid potentiometricallv.

Viva - xoce	16 marks
Note Book	04 marks
Experiment	50 marks
Interval Assignment	20 marks
Day to day interval Assignment	10 marks

M.Sc.
Chemistry
Semester-IV
(Elective-I)

Paper-XIII(A) **CHEE-13 (A)**
Full Marks:70 **Time:3 hrs.**

Organometallic and Bioinorganic Chemistry

UNIT 1 : Alkyls and Aryis of transition metals

Stability of transition metal alkyls, classification of o-bonded hydrocarbyls, general methods of preparation, general characteristics, structure and bonding organocopper compounds.

UNIT 2 : Transition metal – π complexes

Transition metal π – complexes with unsaturated organic molecules / group – alkenes, alkynes, allyl, dienes, dienyl, trienyl, areanes-aynthesis, nature of bonding and structural features, Important reactions, relating to nucleophilic and electrophilic attack on coordinated ligand.

UNIT 3 : Reactions of organometallic compounds

Substitution reactions of carbonyl complexes, Oxidative addition reaction, Reductive elimination reaction, Insertion reaction and Deinsertion reaction.

UNIT 4 : Catalysis by organometallic compounds

General features of catalysis, Types of catalysis, Catalytic steps, Hydrogenation of alkenes (Wilkinson's catalyst), Hydroformylation of alkenes, Ziegler-Natta polymerization of alkenes, Wacker process, Monsanto acetic acid synthesis, Water gas shift reaction, Fischer-Tropsch synthesis. Hydrosilylation, Activation of C-H bond.

UNIT5(a)Metal ions in biological systems

Role of alkali and alkaline earth metals is biological systems,-potassium pump, Active transport of cations across the membrane.

Transport and storage of dioxygen Haem proteins and oxygen uptake, Skucture and function of haemoglobin, myoglobin and haemocyanin.

Electron transfer in biological systems Structure and function of metalloproteins, Vitañiin B_N and mechanism of electron transfer in ferredoxin and cytochrome.

UNt T5(b)Metals in medicines

Metal deficiency and disease, Toxic effect metals, Metal complexes in chemotherapy as drugs and anticancer agents.

BOOK RECOMMENDED

1. Organometallic Chemistry, R.C. MehroYa and A.Singh, New Age International Publishers
2. Organometallic Compounds, I.Kumar, Pragati Prakashan
3. Principles of Bioinorgnanic Chemistry, S.J. Lippard, J.M. Berg Unkv. Science Books

M.Sc.
Chemistry
Semester-IV
(Elective - I)

Paper-XIII (B) **CHEE-13 (B)**
Full Marks:70 **Time:3 hrs.**

Unit 1: Stereochemistry

(A) Stereospecific and stereoselective reactions : Definition and examples.

(B) Review of the stereochemical aspects of SN_1, SN_2, SN_i (Mistsunobu reaction) E_1, E_2, E_{1CB}, E_i, and neighbouring group participation reactions. Role of stereochemistry in rearrangement reactions, Tiffenean – Demjanov rearrangement, Bayer Villiger rearrangement and Beckmann rearrangement and Favroskii rearrangement.

(C) Conformtional analysis of cyclohexanes and decalins including their reactivities of the axially and equatorially substituted conformers.

(D) Conformations of saturated heterocycles : The anomeric effect and the double anomeric effect, stability of 2-substituted pyrones.

Unit 2: Fragmentation reaction :

Definition, Factors affecting fragmentation : Polarization of C-C bond, electron push and pull, Stereochemical requirement. Fragmentation of (a) Three (b) Four (c) six membered rings, Ring expansion by fragmentation –Eschenmoser fragmentation; Beckmann fragmentation.

Unit 3: Asymmetric Synthesis :

Definition, Different methods of asymmetric Synthesis : Resolution, Chiral pool, Chiral auxiliary, Chiral reagent and Chiral catalyst. CBS

reagent, Sharpless asymmetric epoxidation, Sharpless asymmetric dihydroxylation; Baker's yeast.

Unit 4: Synthesis of sinele geometrical isomers of double bonds:

a) Stereoseleotive formation of olefins : The Julia olefination, Stereoselectivity of olefination through E,, E_2 and $E_{ic}B$ mechanism, Witting reaction — E selective and Z selective Witting reaction, Transformation of alynes to Z and E selective alkenes, Synthesis of Z and E selective enolates.

b) Stereospecific formation of olefins : E;, E_2 elimination — Formation of Cisubstituted alkenes, The Peterson reaction. Formation by fragmentation of cyclic compounds.

Unit 5(a)Stereoselective reaction of cyclic systems :

Ster :ose1ective reactions on (a) Four (b) Five (c) Six membered rings with_(i) one trigonal carbon (ii) two or more aigonal carbons (e) bicyclic — Ft sed, bridged and spiro systems (f) more hindred face — (i) teethered nucl zophilic (ii) cyclic Ransition state mediated approach.

Vai ,¿{b)

(. \) Stereospecific alkene transformations: (a) Bromination (b) lodolactonization (c) Epoxidation (d) cis -1, 2 diol and (e) trans l, 2 — diol formation (f) hydroboration.

(3) Stereoselective chiral akene Ransformations : (a) ej› oxidation of chiral aRene Q) alkylation of chiral enolates — Es,planation by the Houk model.

(S) Stereoselective addition of carbonyl group with adjacent stereogenic cenke, Cram's rule, Fekin — Anh mo‹lel, Effect of elecoonegative atoms and chelation on stereoselect vity.

D) Synthesis of Syn and anti aldols: Zimmermann's m‹ del

Ref :-

(1) Principle of Organic Synthesis — Norman & Coxan

(2) Organic synthesis — M.B. Smith

(3) Organic Chemistry — I.L. Finar Vol.-2

(4) Organic Chemistry — Clayden, Greeves, Warren and Wolthers

(5) Organic synthesis The disconnection approach S. Warren

M.Sc.
Chemistry
Semester-IV
(Advanced Quantum Chemistry, Elective - I)

Paper- XIII (C) **CHEE-13 (C)**
Full Marks:70 **Time:3 hrs.**

UNIT 1 Energy of Molecules & Wave Functions

The hydrogen molecule ion, Evaluaiton of U and $9J^2$. Electronic Energy of molecules, Hybrid orbitals — Combinaiton of 1s and one 2p orbital, Combination of 2s and two 2p orbitals, combination of one 2s and three 2p orbitals,

UNIT 2 Hartree Fock Theory

Bom — Oppenheimer Approximation, Slater Condon rules, Hartree-fock Equation, Koopman's Theorem and Roothann's Equation.

UNIT 3 Semi — Empirical Theories

Application of HMO Theory to Benzene, Heteronuclear conjugated systems — Pyrrole and Pyridine. Extended Huckel theory, Th e pariser – Parrpople (PPP) method and its treatment to Ethene and Butadi ene.

UNIT 4 Density Functional Theory

Hohenberg — Kohn Theorems, Kohn-sham Equations Density functional theory and its Applications.

UNIT 5 Scattering Theory

Scattering Cross — section, Scattering length, Law energy scattering Theory, charged particle scattering and coulolnb wave function, Resonance scattering Breit-wigner Formula, Levinson's Theorem. Application of Scattering theory in (a) square well potential, (b) Bound States (c) Resonance (d) Proton — Proton Scattering.

Book Suggested:

1. Quantum Chemistry, T. Veszpremi and M. Feher, Springer.
2. Quantum Chemistry, J.P. Lowe and K.A. Peterson.
3. Elementary Quantum Chemistry, F.A.Pilas, McGraw Hill International Editions.
4. Quantum Chemistry, D.A. Mc Quarrie, Viva Books Pvt. Ltd.
5. Quantum Chemistry, M.R. Awode, S. Chand & Company Ltd.

M.Sc.
Chemistry
Semester-IV
(Elective-II)

Paper-XIV (A) **CHEE-14 (A)**
Full Marks:70 **Time:3 hrs.**

Inorganic Spectroscopy

UNIT 1 : Application IR spectroscopy in the elucidation of structure of metal carbonyls, nitrosyls & dinitrogen complexes and complexes with ambidentate ligands such as NO_2, SCN, CN, etc.\

UNIT 2 : Study of the spectral properties of metal complexes, Splitting of terms of d^1 and d^2 ions in (i) octahedral (ii) tetrahedral and (iii) square planar crystal fields. Orgel diagram, Tanabe-Sugano diagram, Selection rules for electronic transitions, Racah parameters and their calculation, Charge transfer spectra.

UNIT 3 : ESR spectroscopy – Basic principle, Presentation of spectrum. Hyperfine splitting in some simple systems, g- value, Zero field splitting, Krammer degeneracy, Simple applications ESR spectroscopy.

UNIT 4 : Application of ^{1}H, ^{11}B, ^{19}F, ^{13}C and ^{31}P NMR spectroscopy in the elucidation structure of inorganic molecules / ions.

UNIT 5 : Mossbauer spectroscopy – Basic principle, Instrumentation, Spectral parameters – isomer shift, quadrupole splitting, magnetic hyperfine interaction, Applications – (i) oxidation states of metals in their compounds (ii) structure determination (iii) nature of chemical bonding in Prussian blue / Prussiates (iv) covalently bonded molecules (v) magnetically ordered compounds.

BOOKS RECOMMENDED

1. Physical methods in Inorganic Chemistry, R.S. Drago
2. IR Raman Spectroscopy of Inorganic & Coordination compounds, K. nakamoto John Wiley & Sons
3. Electronic Spectrosopy, A.B.P. Lever, Oxford University Press
4. Instrumental methods, Willard, Merritt and Dean, East-West Press
5. Molecular Spectroscopy, C.N. Banwell, TMH

M.Sc.
Chemistry
Semester-IV
(Elective -II)

Paper- XIV(B) **CHEE-14 (B)**
Full Marks:70 **Time:3 hrs.**

Unit 1: Special Techniques of organic synthesis :

Polymer supported reagents and synthesis : introduction properties of polymer support, advantages of polymer supported reagents, choice of polymer, Classification of reactions involving polymers. Synthesis of peptides, solid state Edman degradation, Asymmetric synthesis of atrolactic acid – Example of increased stereoselectivity; use of Ploy-N-bromosuccinimide, polystyrene carbodiimide in organic synthesis, use of Polymer supported photosensitizer and polymer supported phase transfer catalysts and crown ethers.

Unit 2: Microwave induced organic synthesis :

Introduction, microwave oven, reaction, vessel, reaction medium, advantages, limitations, precautions, applications : Synthesis of chalcones (use of solvent), enaminoketones (support catalysis), Knoevenagel reaction (without solvent).

Unit 3: Sonochemistry: The use of ultrasound in organic synthesis :

Introduction, instrumentation physical aspects, types of sonochemical reactions, homogenous reactions, heterogeneous liquid-liquid reactions, heterogeneous solid-liquid reactions, synthetic applications.

Unit 4: Phase –transfer catalyst :

Introduction, factors affecting use of PTC, mechanism of PTC reactions types of PTC, advantages, types of phase transfer catalysed reactions, preparation of phase transfer catalyst, important applications of PTC in organic synthesis.

Unit 5(a)Carbocvclic ring synthesis :

i Three memebered rings, use of caibine intermediates Simmon smith reaction, tise of diazoketone.

ii. Four memebred rings Photochemical (2+2) cycloaddition — regioselectivity, synthesis of ionic reactions, expansion of three membered ring, use of ketenes.

iii. Five memebred rings From 1, 4 dicarbonyl compounds, from 1, 6 — dicarbonyl compounds, Pericyclic rearrangement dienone to cyclopentenone, vinyl cyclopropane to cyclopentene rearrangement. Synthesis via intramolecular radical intermediates cyclization.

iv. Six membered rings . carbonyl condensations, Robinson annelation, Diels — Alder reactions, partial / total reduction of aromatic compounds.

v. Large rings -

a) lnGamolecular cyclization of dinitriles . Ziegler's method.

b) lntramolecular cyclization of diketenes : Blomquist method

c) Acyloin Synthesis.

Unit 5(b)H et é.rocyclic synthesis :

(A) Synthesis of satwated Heterocycles -

Introduction : case of fing closure, Baldwin’s rules for ring closure ReCosynthetic analysis.

Synthesis of three memebered ring‘s, fow membered rings ,:- ionic and pericyclic pathway

M.Sc.
Chemistry
Semester-IV
(Molecular Dynamics ,Elective-II)

Paper- XIV(C) **CHEE-14 (C)**
Full Marks:70 **Time:3 hrs.**

UNIT 1 : **INTRODUCTION TO MOLECULAR REACTION DYNAMICS**

Dynamics of reaction, mechanism of activation, concept and shape of potential energy surfaces, rate of reaction on theoretical Potential energy surfaces, determination of position and properties of the transition state on the surfaces, Dynamic calculation Vs Transition state theory.

UNIT 2 : **KINETICS OF CONDENSED PHASE REACTION**

Factors determining reaction rate in solution, diffusion controlled reactions and activation controlled reactions, collision on solution encounter, Transition state theory in solution, kinetics of ionic reactions, Single and double spherical model, kinetics of dipole-dipole reaction, ion-dipo e reactions, Dependence of rate constant on ionic strength and dielectric constant of the medium, Bronsted — Bjemim equation.

UNIT 3 : **CATALYSIS AND OSCILLATORY BEHAVIOUR**

General mechanism and kinetics of catalytic reactions, Arrhenius interme(iates, Vant Hoff intermediates, Theory of acid-base catalysis, Effect o I salt on acid-base catalysis, Bronsted Catalysis law, linear free energy relationship, Hammet equation, Oscillatory reactions, Lotka-Voltra n odel, B-Z reactions and its mechanism.

UNIT 4 : STUDY OF FAST REACTIONS

Flash photolysis, relaxation technique, NMR method, Molecular beam and shock tube kinetics, stop flow method, Isolnerisation, Photo dissociation and recombination reactions.

UNIT 5 : KINETICS OF ELECTRODE REACTIONS

Faradaic and Non-faradaic curent, Rate law in faradaic process, current density, factors affecting electrode reaction rate, Nernst diffusion layer treatment, Exchange cwrent density, stoichioinetric number and transfer coefficient, energy barrier for inultistep reactions, effect of double layer structure on electrode reaction rates.

UNIT 6 : ELECTRODE DEPOSITION AND CORROSION PROCESS

ElecCobataysis, Electrocatalytic rate, electrocatalysis in redox system, Total dpposition, current density, Time variation of the overpotential and rate determini ng step in electrode deposition.

Referen,ces

1. Advanced Concepts in Physical Chemistry, Kaufman, International Student Edn.
2. Cbemical Kinetics, K.J. Laidler, TMH.
3. Advanced Chemical Kinetics — K.N. Upadhayay
4. Physical Chemitry, Barrow, TMH.
5. Physical Chemistry, Atkins, Oxford
6. Physical Chemistry — A molecular Approach, Viva-books fivt. Ltd.

M.Sc.
Chemistry
Semester-IV
(Laboratory course- Inorganic Chemistry)

Paper-XV **CHEEP-15 (A)**
Full Marks:70 **Time:06 hrs.**

1. Quantitative analysis of a mixture containing not more than three metal ions using volumetric or gravimetric techniques, or 20 marks
   Spectrophotometric determination of metal ions/ anions, or
   Quantitative estimation of major constituents of any one of the following.
   a) Dolomite
   b) Brass
   c) Stainless steel
   d) Bronze
   e) Solder
   Anlysis of two cation system using complexometric method, or
   Determination halide or silver ion by indirect EDTA titration.
2. Synthesis, purification and crystallization of coordination compounds of any of the following Cu(II), Cr(II), Co(II) and Fe(III) ions. 20 marks
3. Analysis of inorganic mixture containing not than six radicals including rare earths, interfering radicals and insoluble compounds 20 marks

Viva - voce	16 marks
Note Book	04 marks
Experiment	50 marks
Interval Assignment	20 marks
Day to day interval Assignment	10 marks

M.Sc.
Chemistry
Semester-IV
(Laboratory course- Organic Chemistry)

Paper-XV **CHEEP-15 (B)**

Full Marks:70 **Time:06 hrs.**

1. **Qualitative analysis**

   Separation, purification and identification of the components of binary mixture of organic compounds

2. **Two step synthesis of organic compounds**

   p- nitroaniline from Acetanilide

   p – Chlorotoluene from p- toluidine

   p – aminoazobenzene from aniline

   Benzilic acid from Benzoin

   Benzanilide from Benzophenone

   Any other two step synthesis may also be carried out.

3. Identification of simple organic compounds by the analysis of their spectral data (u.v., i.r, PMR, CMR and MS Recorded spectral graphs/ data will be supplied.

Viva - voce	16 marks
Note Book	04 marks
Experiment	50 marks
Interval Assignment	20 marks
Day to day interval Assignment	10 marks

M.Sc.

Chemistry

Semester-IV

(Laboratory course- Physical Chemistry)

Paper-XV **CHEEP-15 (C)**

Full Marks:70 **Time:06 hrs.**

1. To determine the critical solution temperature above in Phenol-water system.
2. To determine the Eutectic temperature and the composition of the Eutectic mixture.
3. To determine the order of reaction between I_2 and CH_3COCH_3 catalysed by acids.
4. To study the adsoption of acetic acid on charcoal.
5. To determine K_f of camphor and the molecular wt. of solute by Rast's method.
6. To determine the water equivalent of calorimeter and heat of solution of KCl.
7. To determine the heat of neutralization of HCl against caustic soda and heat of ionization of acetic acid.
8. To determine the basicity of succinic acid thermochemically.
9. To verify Beer's law and to determine the concentration of a coloured solution spectrophotometrically
10. To determine the ionization constant of an indicator spectrophotometrically.

Viva - voce	16 marks
Note Book	04 marks
Experiment	50 marks
Interval Assignment	20 marks
Day to day interval Assignment	10 marks

M.Sc. Chemistry
Semester-IV
(Dissertation/Project)

Paper-XVI **CHEEP-16**

Full Marks:100 **Time:06 hrs.**