SCHEME OF EXAMINATION & DISTRIBUTION OF MARKS

SEMESTER - I

Paper No.	Title of the Paper (s)	Internal Assessment	Term End Exam	Practical	Total Marks
1.	Inorganic Chemistry	20	80		100
2.	Organic Chemistry, Stereochemistry & Pericyclic Reaction	20	80		100
3.	Physical Chemistry- I	20	80		100
4.	Spectroscopy And Mathematics/Biology For Chemists	20	80		100
LAB-I	Organic Chemistry				100
LAB-II	Analytical Chemistry				100
				TOTAL	**600**

SEMESTER - II

Paper No.	Title of the Paper (s)	Internal Assessment	Term End Exam	Practical	Total Marks
1.	Inorganic Chemistry	20	80		100
2.	Organic Chemistry	20	80		100
3.	Physical Chemistry	20	80		100
4.	Spectroscopy, Diffraction Methods & Computer For Chemists	20	80		100
LAB-I	Inorganic Chemistry				100
LAB-II	Physical Chemistry				100
				TOTAL	**600**

SEMESTER - III

Paper No.	Title of the Paper (s)	Internal Assessment	Term End Exam	Practical	Total Marks
COMPULSORY FOR GROUP A, B & C					
1.	Applications Of Spectroscopy	20	80		100
2.	Chemistry Of Bio-Inorganic & Bio-Organic	20	80		100
LAB-I	General (Compulsory)			200	200
OPTIONAL GROUP-A INORGANIC					
3.	Organotrasition Metal Chemistry	20	80		100
4.	Photo inorganic Chemistry	20	80		100
OPTIONAL GROUP- B ORGANIC					
3.	Physical Organic Chemistry	20	80		100
4.	Chemistry Of Heterocyclic Compounds	20	80		100
OPTIONAL GROUP-C PHYSICAL					
3.	Chemistry Of Materials	20	80		100
4.	Advanced Quantum Chemistry	20	80		100
				TOTAL	**600**

SEMESTER - IV

Paper No.	Title of the Paper (s)	Internal Assessment	Term End Exam	Practical	Total Marks
COMPULSORY FOR GROUP A, B & C					
1.	Photochemistry & Solid State Chemistry	20	80		100
2.	Bio-Physical & Environmental Chemistry	20	80		100
OPTIONAL GROUP-A INORGANIC					
3.	Bioinorganic Chemistry & Supra-Molecular Chemistry	20	80		100
4.	Analytical Chemistry	20	80		100
LAB-I	Special			200	200
OPTIONAL GROUP - B ORGANIC					
3.	Medicinal Chemistry	20	80		100
4.	Chemistry Of Natural Product	20	80		100
LAB-I	Special			200	200
OPTIONAL GROUP-C PHYSICAL					
3.	Liquid States	20	80		100
4.	Computation Chemistry	20	80		100
LAB-I	Special			200	200
				TOTAL	**600**
				GRAND TOTAL	**2400**

SEMESTER-II
PAPER –I
INORGANIC CHEMISTRY

Note: - Two questions will be asked from each Unit and student will have the choice to attempt any one question from each unit.

Unit- 1

metal ligand Equilibrium in solution: - Step wise & overall formation constants and their interaction, trends in step wise formation constants, factors affecting the stability of Metal Complexes with reference to nature of metal ion and ligand.

Unit- 2

Reaction mechanism of transition metal complexes:- Energy profile of a reaction, reactivity of metal complexes, Inert and Labile complexes. Kinetic application of valence bond & crystal field theories. Kinetics of octahedral substitution, acid hydrolysis , factors affecting acid hydrolysis. Base hydrolysis, Anation reactions, Reactions without metal ligand bond cleavage, substitution reactions in square planar complexes. The trans effect.

Unit- 3

Metal Complexes:

(A) Mechanism of the substitution reaction, Redox reactions, Electron transfer reactions, mechanism of one electron transfer reaction.

(B) Metal Clusters- **Higher** boranes ,carboranes, metalloboranes and metallocarboranes, Metal carbonyl.

Unit- 4

(A) Metal Carbonyls, Structure and bonding, vibrational spectra of metal carbonyls for bonding and structural elucidation, important reactions of metal carbonyls.

(B) Nitrosyl :- Preparation, bonding, structure & important reactions of transition metal nitrosyl, dinitrogen complexes, tertiary phosphine as ligand.

Unit- 5

Isopoly and Heteropoly Acid & salt: Isopoly acids of transition metals Mo, W,V, Nb , Ta.

Heteropoly acids and salt of Mo, W, Structure of heteropoly acids

Books Suggested:-

1. Advanced Inorganic chemistry: - F.A. Cotton and Wilkinson: John Wiley.
2. Inorganic Chemistry : J.E. Huhey, Harpes & Row
3. Chemistry of the elements: N. N. Greenwood & A Earnshow Pergamon.
4. Inorganic Electronic Spectroscopy – A..B.P. Lever, Elsevier
5. Magnetochemistry - R.L. Carlin, Springer Verlag.
6. Comprehensive Co-ordination Chemistry G. Wilkinson, R.D. Gillars and J.A. McCleverty Pergamon.
7. Chemistry Applications of Group Theory - F.A. Cotton.
1. Group Theory: - Bhattacharya.

SEMESTER-II
PAPER - II
ORGANIC CHEMISTRY
(REACTION MECHANISM)

UNIT- I

Electrophilic substitution reactions:-

Aliphatic electrophilic substitution: - Biomolecular mechanism: SE^2, SE1 and SE_i mechanism, electrophilic substitution accompanied by double bond shifts. Effect of substrates, leaving group and the solvent polarity on the reactivity.

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 susbstrates and electrophiles, Diazonium coupling, Gattermann Koch reaction, vilsmeir reaction.

UNIT- II

Nucleophilic Substitution reactions:-

Aliphatic nucleophilic substitution: The S_N2, S_N1, mixed S_N^1 and S_N^2 and SET mechanism. The neighbourring group mechanism, neighbouring group participation by □ and □ bonds. The SNi mechanism. Nucleophilic substitution at an allylic aliphatic trigonal and at a vinylic carbon . Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium, ambident nucleophile.

Aromatic Nucleophilic substitution: The S_NAr, S_N^1, benzyne and S_{RN}^1 mechanisms, Reactivity-effect of substrate structure, Leaving group and attacking nucleophile. The von Richter, Sommelet-Hauser and Smiles rearrangement.

UNIT- III

Free Radical reactions

Types of free radical reactions, Free radical substitution mechanism, mechanism at an aromatic substrate, neighbouring group assistance, Reactivity for aliphtatic and aromatic substrates at a bridge head. Reactivity in the attacking radicals. The effect of solvents on reactivity. Allylic halogenation (NBS), oxidation of aldehydes to carboxylic acids, auto-oxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salts, Sandmeyer reaction. Free radical rearrangement, Hunsdiecker reaction.

UNIT- IV

(a) Addition to Carbon-Carbon Multiple Bonds

Mechanism and stereo chemical aspects of addition reactions involving electrophiles, Nucleophiles and Free radicals, regio and chemoselectivity, Orientation and reactivity, Addition to cyclopropane ring. Hydrogenation of double and triple bonds. Hydrogenation of Aromatic rings. Hydroborations Michael reaction, epoxidation.

(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 condcnsation reactions involving enolates - Aldol, Knoevenagel, Claisen, Mannich, Benzoin, Perkin and Stobbe reactions, Hydrolysis of ester and amides, Ammonolysis of esters.

UNIT- V

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.

Books Suggested.

1. Advanced Organic Chemistry - Reaction Mechanism and Structure, Jerry March, John Wiley.
2. Advanced Organic Chemistry - F.A. Carey and R.K. Sundberg, Plenum.
3. A Guide Book to Mechanism in Organic Chemistry Peter Sykes- longman.
4. Structure and Mechanism in organic chemistry - C.K. Ingold, Cornell University Press.
5. Organic Chemistry - R.T. Morrison and R.N. Boyed, Prentice - Hall.
6. Modern Organic Reactions H.O. House, Benzamic.
7. Principles of Organic Synthesis - R.P.C. Norman and J.M. Coxon, Blackie Academic and Professional.
8. Reaction Mechanism in Organic Chemistry - S.M. Mukherji and S.P. Singh Macmillan

SEMESTER-II
PAPER - III
PHYSICAL CHEMISTRY
KINETICS & ENERGETICS

UNIT- I

THERMODYNAMICS: Classical Thermodynamics; Brief resume of concepts of laws of thermodynamics, free energy, chemical potential and entropies. Partial molar properties, partial molar free energy, partial molar volume and partial molar heat content and their significances. Determinations of these quantities. Concept of fugacity and determination of fugacity. Non- ideal systems: Excess functions for non-ideal solutions. Activity, Activity coefficient, Debye-Huckel theory for activity coefficient of electrolytic solutions, determination of activity and activity coefficients, ionic strength. Application of phase rule to three component systems, second order phase transitions.

UNIT- II

Statistical Thermodynamics: Concept of distribution, thermodynamic probability and most probable distribution. Ensemble averaging, postulates of ensemble averaging canonical, grand canonical and microcanonical ensembles, corresponding distribution laws (using Lagrange's method of undetermined multipliers). Partition functions - translational, rotational, vibrational and electronic partition functions, calculation of thermodynamic properties in terms of partition function, application of partition function. Heat capacity behavior of solids - chemical equilibria and equilibrium constant in terms of partition functions, Fermi-Dirac statistics, distribution law and application to metal. Bose-Einstein statistics - distribution law and application to helium.

Non Equilibrium Thermodynamics: Thermodynamic criteria for non-equilibrium states, entropy production and entropy flow, entropy balance equations for different irreversible processes (e.g. heat flow, chemical reaction etc.) transformations of the generalized fluxes and forces, non-equilibrium stationary states, phenomenological equations, microscopic reversibility and Onsager's reciprocity relations, electro kinetic phenomena, diffusion electric conduction, irreversible thermodynamics for biological systems, coupled reactions.

UNIT- III

ELECTROCHEMISTRY: Electrochemistry of solutions, Debye-Huckel-Onsager treatment and its extension, ion solvent interactions, Debye-Huckel Jerum mode. Thermodynamics of electrified interface equations, derivations of electro-capillarity, Lippmann equations (surface excess), methods of determination. Structure of electrified interfaces. Guoy-Chapman, Stern, Graham-Devanthan - Mottwatts, Tobin, Bockris, Devanathan models. Over potentials, exchange current density, derivation of Butler-Volmer equation, Tafel plot. Quantum aspects of charge transfer at electrodes- solution interfaces, quantization of charge transfer, tunneling. Semiconductor interfaces - theory of double layer at semiconductor, electrolyte solution interfaces, structure of double layer interfaces. Effect of light a semi-conductor solution interfaces.

UNIT- IV

Electro-catalysis - influence of various parameters, Hydrogen electrode. Bio-electrochemistry, threshold membrane phenomena, Nernst-Plank equation, Hodges-Huxley equation, core conductor models, electrocardiograph. Polarography theory, Ilkovic equation, half wave potential and its significance, Introduction to corrosion, homogenous theory, forms of corrosion monitoring and prevention methods.

UNIT- V

(a) ELECTRON DIFFRACTION-

Scattering intensity vs. scattering angle. Wierl equation, measurement technique, Elucidation of structure of simple gas phase molecules. Low energy electron diffraction and structure of surface.

(b) NEUTRON DIFFERACTION-

Scattering of neutron by solid and liquids, magnetic scattering, measurement techniques. Elucidation of structure of magnetically ordered unit cell.

Book Suggested

1. Physical Chemistry - P.W. Atkins, ELBS
2. Introduction to Quantum Chemistry - A.K.Chandra, Tata McGraw Hill
3. Quantum Chemistry - Ira N.Levine, Prentice Hall
4. Coulson's Valence - R. McWeeny, ELBS
5. Chemical Kientics - K.J. Laidler, McGraw Hill
6. Kinetics and mechanism of chemical transformation - J.Rajaraman and J.Kuriacose; McMillan.
7. Micelles, Theoretical and Applied Aspects - V. Moroi, Plenum.
8. Modern Electrochemistry Vol.I and II - J.O.M. Bockris and A.K.N.Reddy, Plenum.
9. Introduction of Polymer Science - V.R.Gowarikar, N.V.Vishwanathan and J.Sridhar Wiley Easter

SEMESTER-II
PAPER –IV
SPECTROSCOPY, DIFFRACTION METHODS & COMPUTER FOR CHEMISTS

UNIT- I

Electronic Spectroscopy:-

A. Atomic Spectroscopy: - Energy of Atomic orbitals, Vector Representation of momenta & vector coupling, spectra of Hydrogen atom, alkali metal atom.

B. Molecular Spectroscopy: - Energy levels, Molecular orbitals, vibration transition, vibrational progression and geometry of the excited states, Franck-Condon principle, Electronic spectra of polyatomic, molecules, Emission Spectra.

C. Photo Electronic Spectroscopy :- Basic principles, Photo-electic effect Ionisation process, Photo Electron Spectra of simple molecules, E.S.C.A., Chemical Information of E.S.C.A., Auger Electron Spectroscopy-basic idea.

UNIT- II

Magnetic Resonance Spectroscopy:-

A). Nuclear Magnetic Resonance Spectroscopy :- Nuclear Spin, Nuclear resonance, saturation, shielding of magnetic nuclei, chemical shift and its measurements, factors influencing chemical shift, deshielding, spin-spin interaction. Factors influencing coupling constant "J", classification (AB, AMx, ABC, A_2B_2 etc), spin decoupling basic ideas about instruments.

B. Electron Spin Resonance Spectroscopy: - Basic principle, Zero field splitting and orbital energy degeneracy, factors affecting the 'g' value, isotopic and anisotopic hyperfine coupling constant. Spin densities and Applications of ESR

C. Nuclear Quadrupole Resonance Spectroscopy quadrupole nuclear, quadrupole moment electric field gradients, coupling constant splittings, Applications.

D. Photoacoustic Spectroscopy :- Basic principle of photoacoustic spectroscopy (PAS), PAS-gases and condensed-systems, chemical & surface application.

UNIT- III

X-ray Diffraction:-

Bragg's condition, Miller indices, Laue-method, Bragg's method, Debye-scherrer method of X-ray structural analysis of crystals. Index- Reflections identification of unit cell from systematic absences in diffraction pattern structure of simple lattices and X-Ray Intensities structure factor and its relation to intensity and electron density. Phase problem. Description of the procedure for an X-Ray structure analysis, Absolute configuration of molecules.

UNIT- IV

Introduction to Computer and Computer Programming in "C"

Computer Fundamental; - Introduction to Computer organisation. Operating System, DOS, Introduction to UNIX and Window. Computer Languages Principle of programming Algorithm and flow charts.

Programming in C :- Structure of a C Programming, constants, variables, operators and Expressions, data Input & output, decision making, branching and looping statements arrays, well defined functions pointes structure and unions, Format statement. Termination statements. Branching statements such as IF of GO TO statement. LOGICAL variables. Double precision variables. Subscripted variables and DIMENSION. DO statement. FUNCTION and SUBROUTINE. COMMON and DATA statements.

UNIT- V

Programming in Chemistry and use of Computer Programmes.

1. Development of small computer codes Involving simple formulae in Chemistry such as Vander waals Equation, pH Titrations, Kinetic. Radioactive Decays. Evaluation of Lattice Energy and Ionic radie secular equation (within Huckel Theory), Elementry structural features, such as, bond lenths, bond Angle, dihedral angles etc. Of molecules extracted from a database.
2. Introduction and use of computer package MS-Word and Excel. Preparation of graphs and Charts.

Book Suggested for Spectroscopy

1. Modern Spectroscopy - J.M. Hollas Hohnwiley.
2. Applied Electron Spectroscopy for Chemical Analysis Ed. H. Windowi and F.L. Ho Willey interscience.
3. NMR, NQR, ESR and mossbaure spectroscopy in Inorganic chemistry: - R.V. Parish, Ellis Harwood.
4. Physical Method in Chemistry - R.S. Drago, Saunders College.
5. Introduction to Molecular Spectroscopy - G.M. Barrow, Mcgraw Hill.
6. Basic Principle of Spectroscopy- R. Chang Mcgraw Hill.
7. Theory and Application of UV Spectroscopy H.H. Jaffe, and M. Orchin, IBH Oxford.
8. Introduction to Photo electron spectroscopy P.K. Ghosh John Wiley.
9. Introduction to magnetic Resonance. A. Carrington and A.D. Maclachalan Harper & Row.
10. Spectroscopy by Kalsi

Books suggested for Computers

1. Computer and Common Sense: - R. Hunt and J. Shelley Prentice Hall.
2. Computational Chemistry A.C. Norris.
3. Micro Computer Quantam Mechaniscs. J.P. Kilingbeck. Adam Hilger.
4. Computer Programming in fortran IV V. Rajaraman, Prentice Hall.
5. An Introduction to Digital Computer Design, V.Rajaraman and T. Radha Krishanan Prentice Hall.

SEMESTER-II
LABORATORY – COURSE I
INORGANIC CHEMISTRY

Note- Students is accepted to complete all exercises.

1. Qualitative analysis of mixture containing eight radical including some less common metal ions among the following by common method (Preferably semi-micro method)

Group-A

Basic Radicals : - {Ag, Pb, Hg, Cu, Cd, Bi, As, Sb, Sn, Fe, Al, Cr, Zn, Mn, co, Ni, Ba, Sr, Ca, Mg, Na, K, NH_4 ,}

Acid Radicals: - {CO_3, SO_4, SO_3, NO_3, F, Cl, Br, I, NO_2, BO_3, C_2O_4, PO_4}

Group– B

Basic Radicals: - {Ce, Th, Zr, W, Te, Ti, Mo, U, V, Be, Li, Au, Pt.}
Acid Radicals :-{SiO_4, Thiosulphate, Ferrocynide, Ferricyanide, Chromate, Arsenite , Arsenate, Permanganate }

Note – The mixture to be analysed by the students must contain at least one basic and one acid radical from Group B.

2. **Quantitative Analysis:-**
Involving two of the following in ores, alloys or mixture in solution- one by volumetric and other by gravimetric method Ag, Cu, Fe, Cr, Mn, Ni, Zn, Ca, Mg, Chloride, Sulphate.

3. **Estimation of:-**
(A) Phosphoric acid in Commercial ortho phosphoric acid.
(B) Boric Acid in Borax.
(C) Ammonium Ion in Ammonium Salt.
(D) MnO_2 in pyrolusite
(E) Available Chlorine in bleaching powder.
(F) H_2O_2 in commercial sample.

Students are expected to perform at least three exercises From above during laboratory work.

4. Preparation of selected Inorganic compounds and study of their properties by various method including IR, Electronic Spectra, Mossbaur, ESR. Spectra+ Magnetic susceptibility etc.
(i) V0 $(acac)_2$
(ii) cis K $[Cr(C_2O_4)_2(H_2O)_2]$,
(iii) $[Co(NH_3)_6]Cl_3$ trans K $[Cr(C_2O_4)_2(H_2O)_2]$,.$2H_2O$
(iv) Na $[Cr(NH_3)_2(SCN)_4]$
(v) Mn $(acac)_3$
(vi) $K_3[Fe(C_2O_4)_3]$
(vii) Prussian Blue Turnbull's Blue.
(viii) $[Co(NH_3)_6]$ $[Co(NO_2)_6]$
(ix) Hg $[Co(SCN)_4]$
(x) $[Ni(NH_3)_4]Cl_2$, $[Ni(NH_3)_4]Cl_2$
(xi) Ni $(DMG)_2$(xii)$[Cu(NH_3)_4]SO_4$
(xii) $K_3[Cr(C_2O_4)_3].3H_2O$
(xiii) $[Cu(NH_3)_4]SO_4$

SEMESTER-II
LABORATORY COURSE- II
PHYSICAL CHEMISTRY

1. **Adsorption:-**
   a. Verification of Freundlich's Adsorption Isotherm.
   b. To study surface tension – concentration relationship for solutions (Gibbs equation).
2. **Phase Equilibria:**
   a. Determination of congruent composition and temperature of binary system e.g. diphenylamine – benzophenone system.
   b. Determination of glass transition temperature of given salt e. g. $CaCl_2$ conductometrically.
   c. To construct the phase diagram for three component system e. g. chloroform, acetic acid and water.
3. **Chemical Kinetics**
   a. Hydrolysis of an ester/ ionic reactions.
   b. Determination of the velocity constant of hydrolysis of an ester. Determination of effect of (a)change of temperatures, (b)change of concentration of reactants and catalyst and(c)ionic strength of the media on the velocity constant of media.
   c. Determination of the rate constant for the oxidation of iodide ions by hydrogen peroxide
   d. Determination of the primary salt effect on the kinetics of ionic reaction and testing of the Bronsted relationship (iodide ions oxidized by persulphate ion).
4. **Conductometry**
   a. Determination of solubility of sparingly soluble salt (eg, $PbSO_4$, $BaSO_4$) Conductometrically.
   b. Determination of the strength of strong and weak acids in a given mixture conductometrically.
   c. Determination of dissociation constant of weak electrolyte by conductometer.
   d. Determination of velocity constant, Order of reaction and energy of activation for saponification of ethyl acetate by sodium hydroxide.
5. **pH Metry/Potentiometry**
   a. Determination of the strength of strong and weak acid in a given mixture using pH meter/potentiometer.
   b. Determination of dissociation constant of weak acid by pH meter.
   c. Determination of concentration of acid in given buffer solution by pH meter.
   d. Determination of strength of halides in a mixture potentiometrically.
   e. Determination of the valency of mercurous ions potentiometrically.
   f. Determination of the strength of strong acid, weak acids in a given mixture using a potentiometer/ pH meter.
   g. Determination of temperature dependence of EMF of a cell.
   h. Determination of the formation constant of silver- ammonia complex and stoichiometry of the complex potentiometrically.
   i. Determination of activity and activity coefficient of electrolytes.
   j. Determination of thermodynamic constant. $\Delta G, \Delta S$ and ΔH for the reaction by e.m.f. method. $Zn + H_2SO_4 = ZnSO_4 + H_2$
   k. Determination of the dissociation constant of monobasic / dibasic acid
6. **Polarimetry:-**
   Determination of rate constant for hydrolysis/inversion of sugar using a polarimeter. Enzyme kinetic – inversion of sucrose.

7. **Solutions:**
   a. Determination of molecular weight of non-volatile and non- electrolyte/electrolytes by cryoscopy method and to determine the activity coefficient of an electrolyte.
   b. Determination of the degree of dissociation of weak electrolyte and to study the deviation from ideal behaviour that occurs with a strong electrolyte.

Instructions to Practical Examiners in Chemistry.

1. The Board of Examiners - one external and one internal for each branch will meet to decide the exercises and other matter in connection with the conduct of practical examinations.

S.No.	Branch	Marks	Duration
(i).	Lab Course-I Inorganic Chemistry	100	10 hours
(ii)	Lab Course-II Physical Chemistry	100	05 hours

2. Sessional marks will be awarded by External Examiner in consultation with the Internal Examiner.
3. The distribution of marks is as under. Marks for Ex-students are given in parentheses.

For Lab. Course –I (Inorganic Chemistry):

a. Qualitative analysis of mixture containing not more than 8 radicals by semi-microMethod only. 32 (42) marks
b. Quantitative analysis (involving separation) of a solution containing 2 metals, one of these is to be estimated gravimetrically and the other volumetrically. 18 (23) marks
c. (c) Preparation 10 (15) marks
d. (d) Viva voce and manipulation 20 (20) marks
e. (e) Sessional 20 (--) marks

Total 100 (100) marks

For Lab. Course –II (Physical Chemistry):

(a) One practical exercise 60 (80) marks
(b) Viva voice and manipulation 20 (20) marks
(c) Sessional 20 (-) marks

Total 100 (100) marks

As far as possible all the exercises as laid down in the syllabus are set. The scale of marking will be determined by examiners in accordance with the nature of exercises.