M.Sc. Chemistry (Two year Course)

SCHEME OF EXAMINATION w.e.f. 2008-2009

M.Sc. Ist Semester

Paper No.	Code	Nomenclature	Hrs/Week	Max. Marks*
Paper-I	CH-401	Inorganic Chemistry	04	80+20
Paper-II	CH-402	Physical Chemistry	04	-do-
Paper-III	CH-403	Organic Chemistry	04	-do-
Paper-IV	CH-404	General Spectroscopy	03	60+15
		Computer for Chemists	02	

M.Sc. 2nd Semester

Paper No.	Code	Nomenclature	Hrs/Week	Max. Marks*
Paper-V	CH-405	Inorganic Chemistry	04	80+20
Paper-VI	CH-406	Physical Chemistry	04	-do-
Paper-VII	CH-407	Organic Chemistry	04	-do-
	Qualifying	Computer for Chemists	02	80+20
Practicals				
Paper-VIII	CH-408	Inorganic Chemistry Practical	08	100
Paper-IX	CH-409	Physical Chemistry Practical	08	100
Paper-X	CH-410	Organic Chemistry Practical	08	100

Note: 1. Maximum marks of M.Sc. Ist year (i.e. Ist & IInd Semester will be **975 (**Theory 675 marks & practicals 300 marks)

2. Computer for Chemists paper will be held at the end of 2nd Semester and will be Qualifying with pass marks 40%.
3. Practical examinations will be conducted at the end of IInd Semester on three consecutive days and there will be two sessions (Morning & Evening) of 04 Hrs.each. Practical marks will include 10% marks for Viva-Voce and 10% for record files. The payment to the practical examiners will be made on the basis of sessions.

*Each theory paper will include 20% marks as internal assessment as per University rules.

(M.Sc. Final (Three Specializations)

3rd Semester (w.e.f. 2009-2010)

Paper No.	Code	Nomenclature	Hrs/Week	Max. Marks*
Paper-XI	CH-501	Inorganic Special-I/Physical Spl-I/Organic Spl.-I	04	80+20
Paper-XII	CH-502	Inorganic Special-II/Physical Spl-II/Organic Spl.-II	04	-do-
Paper-XIII	CH-503	Inorganic Special-III/Physical Spl-III/Organic Spl-III	04	-do-

4th Semester

Paper No.	Code	Nomenclature	Hrs/Week	Max. Marks*
Paper-XIV	CH-504	Inorganic Special-IV/Physical Spl-IV/Organic Spl-IV	04	80+20
Paper-XV	CH-505	Inorganic Special-V/Physical Spl-V/Organic Spl-V	04	-do-
Paper-XVI	CH-506	Inorganic Special-VI/Physical Spl-VI/Organic Spl-VI	04	-do-
Paper-XVII	CH-507	Inorganic Chemistry Practicals/ Physical Chemistry Practicals/ Organic Chemistry Practicals	08	80
Paper-XVIII	CH-508	Inorganic Chemistry Practicals/ Physical Chemistry Practicals/ Organic Chemistry Practicals	08	80
Paper-XIX	CH-509	Inorganic Chemistry Practicals/ Physical Chemistry Practicals/ Organic Chemistry Practicals	08	140

*Each theory paper will include 20% marks as Internal Assessment as per University rules

1. Maximum marks of M.Sc IInd year (i.e. IIIrd & IVth Semester will be **900** (Theory 600 marks & practicals 300 marks)

2. Practical examinations will be conducted at the end of IVth Semester on three consecutive days and there will be two sessions (Morning & Evening) of 04 hrs. each on each day. Practical marks will include 10% marks for Viva-Voce and 10% for record files.
3. The payment to the practical examiners will be made on the basis of sessions.

M.Sc. Chemistry Ist Semester

Paper I CH-401 Inorganic Chemistry **4 hrs. / Week**

Max. Marks: 80

Time: 3 Hrs.

Note:-*Examiner will set 09 questions and the candidates will be required to attempt 05 questions in all. Out of 09 questions one question will be compulsory containing 08 short answer type questions covering the entire syllabus. Further, examiner will set 02 questions from each section and the candidates will be required to attempt one question from each section. All questions will carry equal marks.*

Section-A

Stereochemistry and Bonding in Main Group compounds: VSEPR theory, dπ -pπ bonds, Bent rule and energetic of hybridization.

(7 Hrs.)

Metal-Ligand Equilibria in solution

Stepwise and overall formation constants and their interactions, trends in stepwise constants, factors affecting 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 spectrophotometry.

(8 Hrs.)

Section-B

Reaction Mechanism of Transition Metal Complexes-I

Inert and labile complexes, Mechanisms for ligand replacement reactions, Formation of complexes from aquo ions, Ligand displacement reactions in octahedral complexes-acid hydrolysis, Base hydrolysis, racemization of tris chelate complexes, electrophilic attack on ligands.

(15 Hrs.)

Section-C

Reaction Mechanism of Transition Metal Complexes-II

Mechanism of ligand, displacement reactions in square planar complexes, the trans effect, theories of trans effect, mechanism of electron transfer reactions – types; outer sphere electron transfer mechanism and inner sphere electron transfer mechanism, electron exchange. (15 Hrs.)

Section-D

Isopoly and Heteropoly Acids and Salts

Isopoly and Heteropoly acids and salts of Mo and W: Structures of isopoly and heteropoly anions.

(7 Hrs.)

Crystal Structures

Structures of some binary and ternary compounds such as fluorite, antifluorite, rutile, antirutile, crystobalite, layer lattices- Cd I_2, Bi I_3; Re O_3, Mn_2O_3, corundum, pervoskite, Ilmenite and Calcite.

(8 Hrs.)

M.Sc. Chemistry Ist Semester

Paper II CH-402 Physical Chemistry 4 hrs. / Week

Max. Marks: 80

Time: 3 Hrs.

Note:-*Examiner will set 09 questions and the candidates will be required to attempt 05 questions in all. Out of 09 questions one question will be compulsory containing 08 short answer type questions covering the entire syllabus. Further examiner will set 02 questions from each section and the candidates will be required to attempt one question from each section. All questions will carry equal marks.*

Section-A

Quantum Mechanics: Postulates of Quantum Mechanics; derivation of Schrodinger wave equation; Max-Born interpretation of ψ and the Heisenberg's uncertainty principle; Quantum mechanical operators and their commutations relation, Hermition operators, (elementary ideas, quantum mechanical operator for linear momentum and angular momentum as Hermition operator). The average value of the square of Hermition operators; commuting operators and uncertainty principle(x & p; E &t); Schrodinger wave equation for a particle in one dimensional box; evaluation of average position, average momentum and determination of uncertainty in position and momentum and hence Heisenberg's uncertainty principle, picorial representation of the wave equation of a particle in one dimensional box and its influence on the kinetic energy of the particle in each successive quantum level, lowest energy of the particle.

Section-B

Thermodynamics: Brief resume of first and second Law of thermodynamics.
Entropy changes in reversible and irreversible processes; variation of entropy with temperature , pressure and volume, entropy concept as a measure of unavailable energy and criteria for the spontaneity of reaction; free energy functions and their significance, criteria for spontaneity of a process; partial molar quantities (free energy, volume ,heat concept), Gibb's-Duhem equation;

Section-C

Chemical Dynamics: Effect of temperature on reaction rates, Rate law for opposing reactions of Ist order and IInd order, Rate law for consecutive Ist order reactions, Collision theory of reaction rates and its limitations, steric factor, Activated complex theory, Ionic reactions: single and double sphere models, influence of solvent and ionic strength, the comparison of collision and activated complex theory.

Section-D

Electrochemistry:

Ion - Ion Interactions: The Debye -Huckel theory of ion- ion interactions: potential and excess charge density as a function of distance from the central ion, Debye Huckel reciprocal length, ionic cloud and its contribution to the total potential, Debye - Huckel limiting law of activity coefficients and its limitations, ion - size effect on potential, ion - size parameter and the theoretical mean - activity coefficient in the case of ionic clouds with finite - sized ions.

Debye - Huckel -Onsager treatment for aqueous solutions and its limitations Debye-Huckel-Onsager theory for non-aqueous solutions, the solvent effect on the mobality at infinite dilution, equivalent conducftivity ($\wedge$) vs. concentration $c^{1/2}$ as a function of the solvent, effect of ion association upon conductivity (Debye- Huckel - Bjerrum equation).

M.Sc. Chemistry Ist Semester

Paper III CH-403 Organic Chemistry 4 hrs. / Week

Max. Marks: 80

Time: 3 Hrs.

Note:-*Examiner will set nine questions and the candidates will be required to attempt five questions in all. Out of nine questions one question will be compulsory containing eight short answer type questions covering the entire syllabus. Further examiner will set two questions from each section and the candidates will be required to attempt one question from each section. All questions will carry equal marks.*

Section-A

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 π-molecular orbitals, annulenes, antiaromaticity, homo-aromaticity, PMO approach. Bonds weaker than covalent, addition compounds, crown ether complexes and cryptands, inclusion compounds, cyclodextrins, catenanes and rotaxanes

Section-B

Stereochemistry : Chirality, elements of symmetry, molecules with more than one chiral centre, diastereomerism. Determination of relative and absolute configuration (octant rule excluded) with special reference to lactic acid, aniline & mandelic acid. Methods of resolution, optical purity, prochirality, enantiotopic and diastereotopic atoms, groups and faces, asymmetric synthesis, cram's rule and its modifications, prelog's rule, conformational analysis of cycloalkanes (upto six membered rings), decalins, conformations of sugars, optical activity in absence of chiral carbon (biphenyls, allenes and spiranes), chirality due to helical shape, geometrical isomerism in alkenes and oximes, methods of determining the configuration.

Section-C

Reaction Mechanism: Structure and Reactivity: Types of mechanisms, types of reactions, thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammond's postulate, Curtin-Hammett principle. Potential energy diagrams, transition states and intermediates, methods of determing mechanisms, isotope effects. Hard and soft acids and bases. Generation, structure, stability and reactivity of carbocations, carbanions, free radicals, carbenes and nitrenes. Effect of structure on reactivity. The Hammett equation and linear free energy relationship, substituent and reaction constants. Taft equation.

Section-D

Purification Techniques: Chromatography: various types of chromatography, principles and applications, counter current distribution, HPLC, electrophoresis

Natural and Synthetic Dyes: Indigo and Alizarin including their structure elucidation, interaction between dyes and fibers, various classes of synthetic dyes including heterocyclic dyes.

Dissachrides: Detailed study of maltose and lactose.

Paper IV CH -404 General Spectroscopy **90 Hrs. (3 Hrs. /week)**

Max. Marks: 60

Time: 3 Hrs.

Note:- *Examiner will set 10 questions and the candidates will be required to attempt 05 questions in all. Out of 10 questions one question will be compulsory containing 08 short answer type questions covering the entire syllabus. Further examiner will set 03 questions from each section and the candidates will be required to attempt atleast one question from each section. All questions will carry equal marks*

Section-A

1. Electromagnetic radiation, interaction of electromagnetic radiation with matter, regions of the
   Spectrum the width and intensity of spectral transitions. Resolving power**.**
2. **Rotational spectra**- The rotation molecules, rotational spectra of diatomic molecules, the spectrum of non-rigid rotator, the effect of isotopic substitutions, rotational spectra of linear and symmetric top polyatomic molecules

3. **Vibrational and Vibrational – Rotational Spectra**: The vibrating diatomic molecule; simple harmonic vibrations, anharmonicity of vibrations, the diatomic vibrating rotator, the interaction of rotations and vibrations, the vibrations of polyatonic molecules, analysis by infrared technique.

4. **Electronics Spectra**: Electronic spectra of idiatonic molecules, vibrational course structure, and rotational fine structure of electronic band, the Frank-Condon principle, intensity of vibrational-electronic band, dissociation energy, the Fortrat diagram.

Section-B

5. **NMR Spectra** Dynamic and magnetic properties of atomic nuclei, nuclear resonance, relaxation processeds, chemical effects in NMR e.g. chemical shift. Absorption intensities, Spin-spin coupling, Elementary idea of time dependents effects in NMR. Instrumentation line diagram.

6. Applications of UV, IR and NMR spectra in the structural elucidation of organic compounds.

Section-C

Electronic Absorption Spectroscopy: Energy levels in diatomic molecules, introduction to electronic transition, Assignment of transitions, Spectra of transition metal complexes, Orgel diagrams, Calculation of Dq and β for Ni^{II} complexes, structural evidence from electronic spectra.

Nuclear Magnetic Resonance: Applications of spin-spin coupling to structure alignment of inorganic compounds, evaluation of reaction rates of fast exchange reactions, the double resonance technique.

Application of infra-red spectroscopy to the determination of inorganic compounds

M.Sc. Chemistry IInd Semester

Paper V CH-405 Inorganic Chemistry **4 hrs. / Week**

Max. Marks: 80

Time: 3 Hrs.

Note:-*Examiner will set 09 questions and the candidates will be required to attempt 05 questions in all. Out of 09 questions one question will be compulsory containing 08 short answer type questions covering the entire syllabus. Further, examiner will set 02 questions from each section and the candidates will be required to attempt one question from each section. All questions will carry equal marks.*

Section-A

Metal-Ligand Bonding

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

(15 Hrs.)

Section-B

Electronic Spectra of Transition Metal Complexes

Spectroscopic ground states, correlation and spin-orbit coupling in free ions for Ist 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, effect of distortion on the d-orbital energy levels. Structural evidence from electronic spectrum, John-Tellar effect, Spectrochemical and nephalauxetic series, charge transfer spectra, electronic spectra of molecular addition compounds.

. **(16 Hrs.)**

Section-C

Magantic Properties of transition metal complexes

Elementary theory of magneto - chemistry, Guoy's method for determination of magnetic susceptibility, calculation of magnetic moments, magnetic properties of free ions, orbital contribution, effect of ligand-field, application of magneto-chemistry in structure determination, magnetic exchange coupling and spin state cross over.

(8 Hrs.)

Metal Clusters

Structure and bonding in higher boranes, Wade's rules, Carboranes, Metal Carbonyl clusters- Low Nuclearity Carbonyl clusters, total electron count (TEC)

(8 Hrs.)

Section-D

Metal -∏ Complexes

Metal carbonyls, structure and bonding, vibrational spectra of metal carbonyls for bonding and structure elucidation, important reactions of metal carbonyls; preparation, bonding, structure and important reactions of transition metal nitrosyl, dinitrogen and dioxygen complexes; tertiary phosphine as ligand.

(15 Hrs.)

M.Sc. Chemistry IInd Semester

Paper VI CH-406 Physical Chemistry 4 hrs. / Week

Max. Marks: 80

Time: 3 Hrs.

Note:-*Examiner will set 09 questions and the candidates will be required to attempt 05 questions in all. Out of 09 questions one question will be compulsory containing 08 short answer type questions covering the entire syllabus. Further examiner will set 02 questions from each section and the candidates will be required to attempt one question from each section. All questions will carry equal marks.*

Section-A

Schrodinger wave equation for a particle in a three dimensional box and the concept of degeneracy of energy levels. Schrodinger wave equation for linear harmonic oscillator, solution by polynomial method, zero point energy and its consequence. Schrodinger wave equation for three dimensional Rigid rotator, energy of rigid rotator, space quantization; Schrodinger wave equaqtion for hydrogen atom, separation of variable in polar spherical coordinates and its solution, principle, azimuthal and magnetic quantum numbers and the magnitude of their values, probability distribution function, radial distribution function and shape of atomic orbitals (s,p & d).

Section-B

Thermodynamics: Brief resume of first and second Law of thermodynamics. Entropy changes in reversible and irreversible processes; variation of entropy with temperature , pressure and volume, entropy concept as a measure of unavailable energy and criteria for the spontaneity of reaction; free energy functions and their significance, criteria for spontaneity of a process; partial molar quantities (free energy, volume ,heat concept), Gibb's-Duhem equation; Classius – Clayperon equation; law of mass action and its thermodynamic derivation. Third law of thermodynamics (Nernest heat theorem, determination of absolute entropy, unattainability of absolute zero) and its limitation. Phase diagram for two completely miscible components systems.

Section-C

Chain reactions: hydrogen - bromine reaction, pyrolysis of acetaldehyde, decomposition of ethane. Photochemical reactions (hydrogen - bromine & hydrogen -chlorine reactions). General treatment of chain reactions (ortho -para hydrogen conversion and hydrogen - bromine reactions), apparent activation energy of chain reactions, chain length, Rice- Herzfeld mechanism of organic molecules decomposition(acetaldehyde) Branching chain reactions and explosions (H_2 - O_2 reaction). Kinetics of (one intermediate) enzymatic reaction : Michaelis - Menton treatment, evaluation of Michaelis 's constant for enzyme - substrate binding by Lineweaver - Burk plot, by Dixon and by Eadie- Hofstae methods. Competitive and non-competitive inhibition.

Section-D

Ion Transport in solutions: Ionic movement under the influence of an electric field , mobility of ions, ionic drift velocity and its relation with current density, Einstein relation between the absolute mobility and diffusion coefficient, the Stokes- Einstein relation , the Nernst -Einstein equation, Waldens rule, the Rate- Process approach to ionic migration , the Rate process equation for equivalent conductivity, total driving force for ionic transport, Nernst - Planck Flux equation, ionic drift and diffusion potential , the Onsager phenomenological equations. The basic equation for the diffusion, Planck- Henderson equation for the diffusion potential.

M.Sc. Chemistry IInd Semester

Paper VII CH-407 Organic Chemistry 4 hrs. / Week
Max. Marks: 80
Time: 3 Hrs.

Note:-*Examiner will set 09 questions and the candidates will be required to attempt 05 questions in all. Out of 09 questions one question will be compulsory containing 08 short answer type questions covering the entire syllabus. Further examiner will set 02 questions from each section and the candidates will be required to attempt one question from each section. All questions will carry equal marks.*

Section-A

Aliphatic Nucleophilic Substtitution: The SN2, SN1, mixed SN1 and SN2, SNi , SN1', SN2' SNI' and SET mechanisms. The neighbouring group mechanisms, neighbouring group participation by π and σ bonds, anchimeric assistance. Classical and nonclassical carbocations, phenonium ions, common carbocation rearrangements. Application of NMR spectroscopy in the detection of carbocations. Reactivity- effects of substrate structure, attacking nucleophile, leaving group and reaction medium.. Ambident nucleophile, regioselectivity. Phase transfer catalysis.

Section-B

.Aliphatic Electrophilic Substitution: Bimolecular mechanisms - SE2 and SEi. The SE1 mechanism, Electrophilic substitution accompained 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 systems. Quantitative treatment of reactivity in substrates and electrophiles. Diazonium coupling, Vilsmeir reaction, Gattermann-Koch reaction.

Aromatic Nucleophilic Substitution: The ArSN1, ArSN2, Benzyne and SRN1 mechanisms. Reactivity – effect of substrate structure, leaving group and attacking nucleophile. The von Richter, Sommelet-Hauser, and Smiles rearrangements.

Section-C

Elimination Reactions: The E2, E1 and E1cB mechanisms . Orientation of the double bond . Reactivity –effects of substrate structures, attacking base, the leaving group and the medium. Mechanism and orientation in pyrolytic elimination.

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.
Hydrogenation of double and triple bonds, hydrogenation of aromatic rings. Hydroboration. Michael reaction. Sharpless asymmetric epoxidation.

Section-D

Addition to Carbon-Hetero Multiple Bonds: Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acids, esters and nitriles. Addition of Grignard reagents, organozinc and organolithium reagents to carbonyl and unsaturated carbonyl compounds. Wittig reaction. Mechanism of condensation reactions involving enolates – Aldol, Knoevenagel, Claisen, Mannich, Benzoin, Perkin and Stobbe reactions. Hydrolysis of esters and amides, ammonolysis of esters.

Paper VIII CH-408 Inorganic Chemistry Practical 240 Hrs. (8Hrs./Week)

Max. Marks: 100
Time: 8 Hrs.

1. Qualitative Analysis:
   a) Less common metal ions- Tl, Se, Te, Mo, W, Ti, Zr, U&V
   b) Insolubles- Oxides(WO_3, Silica, Alumina); Sulphates(Lead Sulphate, Barium Sulphate Strontium Sulphate and Calcium Sulphate); Halides(Calcium fluoride and silver halides)

   (2 less common metal ions and 1 insoluble to be given) (30 Marks)
2. Quantitative Analysis:
   a) Separation and determination of two metal ions such as Ag- Cu, Cu- Ni, Cu- Zn, Ni- Zn, Cu-Fe etc. involving volumetric and gravimetric methods. (35 Marks)
   b) Determination of Ferrous, Oxalate, Nitrite etc. by Cerimetry (15 Marks)
3. Viva-Voce (10 Marks)
4. Note Book (10 Marks)

Paper IX CH-409 Physical Chemistry Practical 240 Hrs. (8Hrs./Week)

Max. Marks: 100

Time: 8 Hrs.

1. Conductometry

(i) Determination of cell constant
(ii) NaOH vs. HCl titration.
(iii) NaOH vs. Oxalic acid titration
(iv) NaOH vs. CH_3COOH titration.
(v) $AgNO_3$ vs. KCl titration.
(vi) $Ba(NO_3)_2$ vs. Na_2SO_4 titration.

2. Potentiometry

(i) NaOH vs. HCl titration.
(ii) NaOH vs.Oxalic acid titration.
(iii) NaOH vs. CH_3COOH titration
(iv) $AgNO_3$ vs. Kcl titration.
(v) $KMnO_4$ vs. Mohr's Salt/ $FeSO_4$ titrations.

3. pH metry

(i) NaOH vs. HCl titration.
(ii) NaOH vs. Oxalic acid titration.
(iii) NaOH vs. CH_3COOH titration.

4. Thermochemistry

(a). Determination of heat of neutralisation
(i) NaOH vs. HCl .
(ii) NaOH vs. CH_3COOH
(iii) NaOH vs. Oxalic acid.

(b) Determination of Heat of solution and Heat of hydration of $BaCl_2$ and $CuSO_4$

5. Chemical Kinetics

(i) To study kinetics of hydrolysis of an ester in the presence of acid
(ii) To compare the relative strength of acids(HCl and H_2SO_4
(iii) To determine the temperature coefficient for the Ist order reaction.

1. Refractometry

(i) Determination of molar refractivity of the given liquid.
(ii) To determine percentage composition of liquids in the given binary mixture.

6. Viva-Voce (10 Marks)

7. Note Book (10 Marks)

Paper -X CH-410 Organic Chemistry Practical 240 Hrs. (8Hrs./Week)

Max. Marks: 100

Time: 8 Hrs.

1. Qualitative Analysis (45 Marks)

Separation, purification and identification of compounds of binary mixtures by chemical tests and checking purity of individual components using TLC. IR spectra to be used for functional group identification.

2. Organic synthesis

Two Step Preparations:

(35 Marks)

Preparation of

p-nitroaniline from p-bromoaniline

anthranilic acid from phthalic anhydride

p-bromoacetanilide from aniline.

p-nitroacetanilide from aniline

sym-tribromoaniline from aniline

2,4-dinitrophenylhydrazine from chlorobenzene

2,5-dihydroxy acetophenone from hydroquinone

3. Viva-Voce (10 Marks)

4. Note Book (10 Marks)

Computers for Chemists **60 Hrs (2 Hrs/week)**

Max. Marks :100

Time : 2 hrs.

Essentials of Computer:

Historical Evolution of Computers, Block diagram of a Computer and functions of various units; Classification of Computers; Input/Output devices (Display Devices, Printers, etc.) Memories: RAM, ROM, Cache Memory, Virtual memory; Mass-storage Media: Magnetic Disks, Magnetic Tapes and Optical Disks; Batch processing systems, Time sharing systems, Multiprocessor, Parallel Processing Systems.

Introduction to Programming languages: 1 GL to 5 GL languages. Software and its types; Operating System with DOS as an example, Introduction to UNIX and Windows.

Overview of: Information Technology (IT), Data Communication, Computer Networks (LAN, WAN and MAN) and their applications, Introduction to Internet and Intranet technology.

Computer Applications: Scientific, Business, Research, Sports, Medicine & Health Care, Engineering, Teaching etc.

Problem Solving: Problem Identification, Analysis, flowcharts, Decision Tables, Pseudo codes and algorithms, Program Coding, Program Testing and Execution.

Computer Programming Language (FORTRAN Language) :

Elements of the computer language. Constants and variables. Operations and symbols. Expressions. Arithmetic assignment statement. Input and Output. Format statement. Termination statements. Branching statements such as IF or GO TO statement. LOGICAL variable. Double precision variables. Subscripted variables and DIMENSION. DO statement. FUNCTION and SUBROUTINE. COMMON and DATA statements.

A brief introduction to C language.

Books Suggested

1 Computers and Common Sense, R. Hunt and J. Shelley, Prentice Hall.
2 Computational Chemistry, A.C. Norris.
3 Microcomputer Quantum Mechanics, J.P. Killngbeck,Adam Hilger.

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IIIrd Semester

Paper XI CH-501 Inorganic Special-I 4 hrs. / Week
(Instrumental Techniques) *Max. Marks: 80*
Time: 3 Hrs.

Note:-*Examiner will set nine questions and the candidates will be required to attempt five questions in all. Out of nine questions one question will be compulsory containing eight short answer type questions covering the entire syllabus. Further examiner will set two questions from each section and the candidates will be required to attempt one question from each section. All questions will carry equal marks.*

Section-A

Vibrational Spectroscopy: Symmetry and shapes of AB_2, AB_3,AB_4.AB_5 and AB_6, modes of bonding of ambidentate ligands, ethylenediamine and diketonate complexes, application of resonance Raman Spectroscopy particularly for the study of active sites of metalloproteins as myoglobin and haemoglobin.

15 Hrs.

Section-B

Electron Spin Resonance Spectroscopy: Principle, Presentation of the spectrum, hyperfine coupling, hyperfine splitting in various structures, Factors affecting magnitude of g, zero field splitting and Kramer's degeneracy, Applications to transition metal complexes having one and more than one unpaired electron, applications to inorganic free radicals, study of electron exchange reactions.

15 Hrs.

Section-C

Mossbauer Spectroscopy: Basic Principles, spectral display, isomer shift, factors affecting the magnitude of isomer shift, quadrupole and magnetic hyperfine interaction, applications of technique to the study of bonding and structure of Fe^{2+}, Fe^{3+} ; Sn^{2+} and Sn^{4+} compounds; detection of oxidation states, nature of M-L bond,.

(8 Hrs.)

Mass Spectrometry: Principle, representation, interaction of molecule with high energy electrons, interpretation of mass spectrum, effect of isotopes on appearance of mass spectrum; applications- finger print application, molelcular weight determination, evaluation of heat of sublimation of high melting solids. **(7 Hrs.)**

Section-D

Atomic Absorption Spectroscopy: Principle, instrumentation, applications, sensitivity and detection limits, interferences in AAS and their elimination. **(7 Hrs.)**

Principle and Applications of TGA and DTA **(8 Hrs.)**

IIIrd Semester

Paper XII CH-502 Inorganic Special-II 4 hrs. / Week
(Nuclear & Radiochemistry) *Max. Marks: 80*
Time: 3 Hrs.

Note:-*Examiner will set nine questions and the candidates will be required to attempt five questions in all. Out of nine questions one question will be compulsory containing eight short answer type questions covering the entire syllabus. Further examiner will set two questions from each section and the candidates will be required to attempt one question from each section. All questions will carry equal marks.*

Section-A

Nuclear Binding Energy: Justifications and applications; nuclear stability rules and decay of unstable nuclei.

Nuclear Structure: Nuclear forces; liquid drop model, Shell Model and collective model. (15 hrs.)

Section-B

Interaction of Radiation with matter: Physical and chemical effects of radiation on matter (photoelectric effect, Compton effect and pair production). (7 hrs.)

Radiochemical Techniques:

NAA - Principle, Application and Limitation
IDA - Principle, Application and Limitation
Radiometric titrations. (8 hrs.)

Section-C

Detection of Nuclear Radiation: Various methods of detecting nuclear radiations, Gas-filled counters – Ionization chamber; Proportional counter and G.M. counters. Scintillation detectors; Solid state detectors. (15 hrs.)

Section-D

Nuclear Reactions: Energetics of nuclear reactions; various types of nuclear reactions including photonuclear, thermonuclear and spallation reactions; mechanism of nuclear reaction by compound nucleus model.
Nuclear fission – Fission probability; energy release; theories of fission.

Nuclear Fussion: Brief idea about breeder reactors,; accelerators and cyclotron.
(15 hrs.)

IIIrd Semester

Paper XIII CH-503 Inorganic Special-III
(Bio-Inorganic Chemistry and Environmental Chemistry)

4 hrs. / Week
Max. Marks: 80
Time: 3 Hrs.

Note:-*Examiner will set nine questions and the candidates will be required to attempt five questions in all. Out of nine questions one question will be compulsory containing eight short answer type questions covering the entire syllabus. Further, examiner will set two questions from each section and the candidates will be required to attempt one question from each section. All questions will carry equal marks.*

Section-A

Metal Ions in Biological Systems: General survey of essential and trace metals, Disturbing factors in metabolic process and causes of diseases, different classes of drugs. (5 Hrs.)

Alkali and alkaline earth metals in biological systems: Ionophores, active transport of cations across membranes, sodium pump, Calcium pump, Calcium carriers, role of carriers in muscle contraction, blood clotting and hormones. (7 hrs.)

Interaction of metal ions with Nucleotides: metal ions in nucleotide systems, effect of metal ions on nuclei acids. (3 hrs.)

Section-B

Oxygen carriers: Porphyrins, metalloporphyrins, Hemoproteins, structure and functions of hemoglobin and myoglobin, synthetic oxygen carrier model systems (6 hrs.)

Nitrogen fixation: Biological nitrogen fixation, Nitrogenase, model for nitrogenase, metal-N_2 complexes, photosynthesis and chlorophyll. (6 hrs.)

Metal transport and storage: Transferrin, Ferritin, Siderophores (3 hrs.)

Section-C

Metalloenzymes*:*

Zinc Enzymes – Carboxypeptidase & Carbonic anhydrase

Iron Enzymes – Catalase, peroxidase & cytochrome P- 450

Copper Enzymes – Superoxide dismutase, blue copper- proteins

Coenzymes – Vitamins B_{12} (15 hrs.)

Section-D

Environmental Chemistry: Atmosphere: Chemical composition of atmosphere, atmospheric structure, Earth's radiation balance; oxides of N,C,S and their effects, Green house effect, acid rain, photochemical smog , air quality standards, depletion of ozone, particulate matter in atmosphere , mechanism of aerosol formation in air,Noise pollution and their health hazards.

IVth Semester

Paper XIV CH-504 Inorganic Special-IV
(Organotransition metal Chemistry)

4 hrs. / Week
Max. Marks: 80
Time: 3 Hrs.

Note:-*Examiner will set nine questions and the candidates will be required to attempt five questions in all. Out of nine questions one question will be compulsory containing eight short answer type questions covering the entire syllabus. Further examiner will set two questions from each section and the candidates will be required to attempt one question from each section. All questions will carry equal marks.*

Section-A

Introduction and Classification of organometallic compounds by bond types viz. covalent, ionic, electron deficient and cluster compounds. **(7 Hrs.)**

Alkyls and Aryls of Transition Metals: Types, routes of synthesis, stability and decomposition pathways, organocopper in organic synthesis. **(8 Hrs.)**

Section-B

Transition Metal π–Complexes: Transition metal π–complexes with unsaturated molecules- alkenes, alkynes, allyl, & dienyl(metallocene) complexes, preparation, properties and nature of bonding and structural features, important reactions related to nucleophilic and electrophilic attack on ligands and to organic synthesis.

(15 Hrs.)

Section-C

Compounds of Transition Metal-Carbon Multiple Bonds: Transition metal- carbene complexes: Fischer type and Schrock type carbene complexes, their synthesis, reactions and structures & bonding; Transition metal-carbyne complexes: their synthesis, reactions and structural features.

(15 Hrs.)

Section-D

Fluxional Organometallic Compounds: Fluxionality & dynamic equilibria in compounds such as acyclic alkenes,σ-bonded and π–bonded cyclic alkenes, rotation of ligands on metals, ligand scrambling on metals.

(7 Hrs.)

Applications of Transition metal Organometallics as Catalysts: Zeigler-Natta polymerization ; homogeneous catalytic hydrogenation; alkene hydrogenation-Wilkinson Catalyst; Oxidation of olefins-Wacker's process; hydroformylation of olefins – the oxo process. **(8 Hrs.)**

IVth Semester

Paper XV CH-505 Inorganic Special-V
(Electro Analytical Chemistry)

4 hrs. / Week
Max. Marks: 80
Time: 3 Hrs.

Note:-*Examiner will set nine questions and the candidates will be required to attempt five questions in all. Out of nine questions one question will be compulsory containing eight short answer type questions covering the entire syllabus. Further examiner will set two questions from each section and the candidates will be required to attempt one question from each section. All questions will carry equal marks.*

Section-A

Electrons at and across interfaces, Electro-chemical and chemical reactions**,**.

Basic principles, residual current, migration current, diffusion current and limiting current, saturated calomel electrode(SCE) and dropping mercury electrode(DME). Ilkovic equation, Koutecky equation for diffusion current, Polarographic waves(anodic and cathodic), Half wave potentials. Oxygen interference, maxima, function of supporting electrolyte, **(15 Hrs.)**

Section-B

Determination of stability constants of complexes (reversible systems only) by D.C.Polarography, Catalytic hydrogen wave. Principles of Amperometric titrations, types of titration curves, apparatus and techniques.

Hanging mercury drop electrode, rotating droping mercury electrode, platinum electrodes(RPE), Gold electrode, carbon paste electrode, glassy carbon electrode and graphite electrode. **(15 Hrs.)**

Section-C.

Super imposed a.c. Polarography, voltametry in quiet and stirred solution with electrode other than mercury, square-wave polarography, normal and differential pulse polarography, chronopotentiometry, chronoamperometry and coulometry.

(15 Hrs.)

Section-D

Theory of anodic stripping voltametry, concentration process, rest period, stripping process, Cathodic stripping voltametry, Anodic deposition, Cathodic redissolution, Experimental and applications of above system to Inorganic systems. Theory of ion selective electrodes, Experimental and applications of ISE to Inorganic systems.

(15 Hrs.)

IVth Semester

Paper XVI CH-506 Inorganic Special-VI
(Medicinal Aspects of Inorganic Chemistry)

4 hrs. / Week
Max. Marks: 80
Time: 3 Hrs.

Note:-*Examiner will set nine questions and the candidates will be required to attempt five questions in all. Out of nine questions one question will be compulsory containing eight short answer type questions covering the entire syllabus. Further, examiner will set two questions from each section and the candidates will be required to attempt one question from each section. All questions will carry equal marks.*

Section-A

Metals in Medicine: Biochemical bases of essential metal deficient diseases; Iron, copper and zinc deficiencies and their therapies, carcinogens and carcinostatic agents, zinc in tumour growth and inhibition, anticancer activity and mechanism of platinum complexes, anticancer activity of Rhodium, copper and Gold complexes, anti cancer activity of Selenium, antibacterial and antiviral properties of metal complexes, polyamino carboxylic acids and polyethylene amines as chelating drugs. (16 hrs.)

Section-B

Miscellaneous applications of Inorganic compounds as medicines: Drugs in hypo and hyper activity of thyroids, Inorganic drugs in dental carries, clinical disorders of alkali and alkaline earth metals and their remedies, lithium drugs in psychiatry.

(7 hrs.)

Heavy metals in Biological systems: 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. (7 hrs.)

Section-C

Ligand Therapy: Ligand induced toxicity, interference with haemoglobin in oxygen transport system, intefererence with metallo-enzymes, beneficial effects of ligand chelation; carcinogenic ligands, carcinostatic ligands, alkylating agents as anticancer drugs, Thiosemicarbazones as anticancer drugs, macrocyclic antibiotic ligands and prodable mechanism of the drug, antiviral activity of chelating agents, aspirin chelation, drugs where chelation and therapeutic activity are unrelated. (15 hrs.)

Section-D

Hydrosphere: Chemical composition of water bodies-lakes, streams & rivers; water quality parameters- dissolved oxygen, BOD, water quality standards; Purification and treatment of water.

(8 hrs.)

Radio pharmacology, nuclear medicines, radioiodine-131, technetium-99m, gallium and indium scan. (7 hrs.)

Paper-XVII CH-507 Inorganic Chemistry Practical

8Hrs./Week
Max. Marks: 80
Time: 8 Hrs.

Preparation of selected Inorganic compounds/complexes and their characterization using techniques/methods such as elemental analysis, conductance measurement, molecular weight determination, magnetic susceptibility measurements, infrared, UV, visible, Mossbauer and ESR spectra etc. Handling of air and moisture sensitive compounds.

i) Chromous Acetate
ii) $Hg[Co(SCN)_4]$
iii) $Ni(dmg)_2$
iv) $[Cu(NH_3)_4]SO_4.H_2O$
v) $[Ni(NH_3)_6]Cl_2$
vi) $K_3[Fe(C_2O_4)_3]$
vii) $VO(acac)_2$
viii) $Mn(acac)_3$
ix) Prussian blue
x) $[Co(NH_3)_5Cl]Cl_2$; $[Co(NH_3)_5NO_2]Cl_2$; $[Co(NH_3)_5ONO]Cl_2$
xi) $K_3[Al(C_2O_4)_3]$
xii) $[Ni(en)_3]S_2O_3$ etc.

Paper XVIII CH-508 Inorganic Chemistry Practical

8 Hrs. / week
Max. Marks: 80
Time 8 Hrs.

Two experiments from the following to be given:

1. Estimation of metal ions by atomic absorption spectrophotometry and Flame Photometry.
2. Spectrophotometric determination of Fe, Ni,Mn,Cr,V,Ti and fluoride, Nitrate and phosphate etc.
3. Determination of pK value of an indicator Spectrophotometrically.
4. Study of Complexation (Stoichiometry and stability constant) between Fe-thiocynate, Fe-Phenanthroline and Cu- ethylenediamine by Job's method/ slope ratio method.
5. Polarographic determination of metal ions such as Zn,Cd, Mg, Tl etc.(including mixtures). Amperometric titrations.

(2×40 Marks)

Paper XIX CH-509 Inorganic Chemistry Practical

8Hrs. /Week
Max. Marks: 140
Time: 8 Hrs.

1. Separation of cations and Anions by Column Chromatography- Ion exchange.
(40 Marks)
2. One Experiment from the following:
   a) Conductometrically – Composition of mixture of weak and strong acids, precipitation and displacement titrations.
   b) pH – metry – Composition of mixture of strong and weak acids, pKa value of organic acids.
   c) Potentiometry- redox titrations, precipitations, simultaneous determination of Halide ions.
   d) Ion – selective electrodes- F, Ca, Na, K etc.

(40 Marks)

3. Viva-Voce **(30 Marks)**
4. Record file **(30 Marks)**

IIIrd Semester

Paper XI CH-501 Physical Special-I 4 hrs. / Week

Max. Marks: 80

Time: 3 Hrs.

Note:-*Examiner will set nine questions and the candidates will be required to attempt five questions in all. Out of nine questions one question will be compulsory containing eight short answer type questions covering the entire syllabus. Further examiner will set two questions from each section and the candidates will be required to attempt one question from each section. All questions will carry equal marks.*

Section-A

Electrifield Interfaces: Thermodynamics of electrified interfaces: electrocapillary thermodynamics, non-polarizable interface and thermodynamic equilibrium, fundamental thermodynamic equation of polarizable interfaces, determination of excess charge density on the electrode, electrical capacitance and surface excess of the interface, potential of zero charge, Helmholtz-Perrin model, Gouy - Chapman model and Stern model of electrified interfaces.

Section-B

Ionic Liquids: The thermal dismantling of an ionic lattice, characteristics of ionic liquids, the fundamental problems in the study of pure liquid electrolytes, models of simple ionic liquids: lattice oriented models (the vacancy model, the hole model) , quantification of the hole model, the Furth approach to the work of hole formation, distribution function for the sizes of the holes and the average size of a hole.

Electrodics: Rate of charge- transfer reactions under zero field, under the influence of an electric field, the equilibrium exchange current density, the non-equilibrium drift-current density (Butler - Volmer) equation. Some general and special cases of Butler- Volmer equation, the high-field and low-field approximations, physical meaning of the symmetry factor (β), a preliminary to a second theory of β , a simple picture of the symmetry factor and its dependence on overpotential. Polarizable and non-polarizable interfaces.

Section-C

Adsorption : Surface tension, capillary action, pressure difference across curved surface (Leplace equation), Gibb's adsorption equation and its applications, determination of BET equation and its application for the determination of surface area; surface active agents and their classification, concept of micelles, critical micelle concentration (cmc), determination of cmc by conductivity and surface tension methods; factors affecting cmc, counter - ion binding to micelles, thermodynamics of micellization

Section-D

Chemical Dynamics: Study of fast reactions, Flow methods, Relaxation method, Flash photolysis and shocktube method. Theoriesof unimolecular reactions: Lindemann's theory, Hinshelwoods treatment, R.R.K. and R.R.K.M. theories,The theory of absolute reaction rates, potential energy surfaces, activation energies, London— Eyring - Polanyi method for the calculation of energy of activation.

IIIrd Semester

Paper XII CH-502 Physical Special-II 4 hrs. / Week
Max. Marks: 80
Time: 3 Hrs.

Note:-*Examiner will set nine questions and the candidates will be required to attempt five questions in all. Out of nine questions one question will be compulsory containing eight short answer type questions covering the entire syllabus. Further examiner will set two questions from each section and the candidates will be required to attempt one question from each section. All questions will carry equal marks*

Section-A

Statistical Thermodynamics: Concept of distribution, thermodynamic probability and most probable distribution; canonical, grand canonical and micro canonical ensembles. Maxwell - Boltzmann statistics, Statistical thermodynamic formulation of Maxwell - Boltzmann distribution law, Maxwell - Boltzmann law of distribution of energy and evaluation of average velocity, root mean square velocity; law of equipartition of energy; Partition function and its factorization, relationship of atomic and molar partition function to thermodynamic properties(I) internal energy (ii) entropy (iii) Gibb's free energy (iv) heat contant (v) work function (vi) pressure (vii) heat capacity at constant volume. Derivation of equation of state for a mono atomic ideal gas.

Section-B

Translational partition function, calculation of absolute entropy of an ideal monoatomic gas, Seckure -Tetrode equation, Vibrational , Rotational, & electronic partition function of diatomic molecules, Derivation of expressions for transitional ,vibrational, rotational, electronic energy; expressions for entropy, Gibbs free energy, work function due to transitional, vibrational and rotational motion of a molecule. Effect of change of zero point energy on partition function and also on thermodynamic properties like internal energy, Gibbs free energy, enthalpy, work function & entropy. Chemical equilibrium and equilibrium constant in terms of partition functions, Free energy function.

Section-C

Quantum mechanical treatment of Helium atom and the failure of rigorous quantum mechanical method, need of approximate methods, first order perturbation theory (excluding time dependent), variation principle. Application of first order perturbation and variation principle to evaluate ground state of helium atom. Applicability of perturbation theory to an electron in a one dimensional box under the influence of electric field.

Section-D

Valance bond method, valance bond method to hydrogen, hydrogen molecule ion (their symmetric and anti symmetric solution without actual valuation of various integrals, energy of molecular hydrogen system, LCAO-MO approximation, refined treatment of hydrogen molecules Concept of resonance and its role in the stability of hydrogen molecule ion, electron spin, pauli's exclusion principle, hybridization.

IIIrd Semester

Paper XIII CH-503 Physical Special-III 4 hrs. / Week

Max. Marks: 80

Time: 3 Hrs.

Note:-*Examiner will set nine questions and the candidates will be required to attempt five questions in all. Out of nine questions one question will be compulsory containing eight short answer type questions covering the entire syllabus. Further examiner will set two questions from each section and the candidates will be required to attempt one question from each section. All questions will carry equal marks*

Section-A

Spin Resonance Spectroscopy: Spin and an applied field; the nature of spinning particles, interaction between spin and magnetic field, Larmor precession, population of energy levels. Nuclear MagneticResonance Spectroscopy; Hydrogen Nuclei, the chemical shift, the coupling constant, coupling between several nuclei, analysis by NMR technique, exchange phenomena, simplication of complex spectra.

Section-B

Electron spin resonance spectroscopy; the theory of E.S.R. the position of E.S.R. absorption, the g factor, the fine and hyperfine structures of E.S.R. absorption. Applications of E.S.R. spectroscopy.

Moss Bauer Spectroscopy: The theory of Moss-Bauer spectroscopy, the chemical shift quadrupole effects, the effect of magnetic field, application of Moss-Bauer spectroscopy.

Section-C

Introduction: Definition of corrosion, importance and cost of corrosion classification of corrosion

Electrochemistry of Corrosion: Electrode reactions, electrode potentials, electrochemical cell formation, Nernst equation, exchange current density, polarization of electrode (resistance, concentration and activation), mixed potential theory, polarization diagrams, pourbaix diagrams, corrosion rate expression and weight loss method for corrosion rate, galvanic series. Electrochemical techniques to study corrosion – Galvanostatic and potentiostatic techniques, Stern –Geary equation, Tafel slopes, measurement of corrosion potential and corrosion current density, Tafel extrapolation and Linear polarization resistance methods, recording and interpretation of anodic and cathodic polarization curves.

Section-D

Kinetics of Passivity: Introduction , electrochemical behaviour of active/passive metals, Flade potential, criteria for selecting a metal exhibiting passivity, factors influencing electrochemical passivity and corrosion rate, theories of passivity.

Protection Methods against Corrosion: Change of metal, design improvement, change of environment, anodic protection, cathodic protection and protective coatings.

Corrosion inhibitors: classification, mechanism, selection of corrosion inhibitors, inhibition efficiency and factors influencing inhibition efficiency, measurement of inhibition efficiency.

IVth Semester

Paper XIV CH-504 Physical Special-IV 4 hrs. / Week
Max. Marks: 80
Time: 3 Hrs.

Note:-*Examiner will set nine questions and the candidates will be required to attempt five questions in all. Out of nine questions one question will be compulsory containing eight short answer type questions covering the entire syllabus. Further examiner will set two questions from each section and the candidates will be required to attempt one question from each section. All questions will carry equal marks.*

Section-A

Applications of Electrochemistry: The maximum intrinsic efficiency, actual efficiency and current - potential relation in an electrochemical energy converter, factors influencing the electrochemical energy conversion, the power output of an electrochemical energy converter. Electrochemical electricity generators (fuel cells), brief idea about H_2- O_2, hydrocarbon - air, and natural gas & CO -air fuel cells. Electricity storage: some important quantities in electricity storage (electricity storage density, energy density, power), desirable conditions for an ideal strorer , storage of electricity using the lead-Acid battery, dry cell, silver-zinc cell and Sodium- Sulfur cell, Amperometric titrations determination of activation energy for an irreversible electrode process.

Section-B

Polarography: General principles of polarography, the limiting current, diffusion current, derivation of Ilkovic equation, consequences of the Ilkovic equation, Koutecky's equation for diffusion current, half -wave potential, equations for reversible cathodic, anodic, and cathodic-anodic waves, analysis of reversible polarographic wave, factors affecting the half- wave potential, reversible processes controlled by diffusion of complex ions, $(Me^{n+} + pX^{m-} \Leftrightarrow [MeX_p]^{(mp-n)-}$, reversible reduction of organic substances (quinone - quinol system).

Irreversible electrode processes : An approximate treatment of a slow electrode process and regorous treatment of a slow electrode process, irreversible reduction of complexes, polarography of organic substances, polarographic coulometry at constant potential, determination of number of electrons by analysis of the decrease in the limiting current.

Section-C

Polymers: Classification of polymers and polymerisation, condensation and addition polymers, kinetics of condensation (step-wise) polymerisation, size distribution in linear condensation polymers, molecular size control, degree of polymerization; mechanism of vinyl radical polymerisation, molecular weight and its determination, effect of temperature and pressure on chain polymerisation, stereochemistry of polymer chain & stereo regular polymerisation, Ionic polymerisation (similarities and contrast), kinetics of cationic, anionic polymerisation, kinetics of copolymerisation, criteria for polymer solubility; Mass number and Mass average molecular weight, determination of molecular weight of polymers by osmometry, viscometry, light scattering and sedimentation method.

Section-D

Polymers:

Statistical method of biopolymers: Chain configuration of polymer chains, statistical distribution of end to end dimensions (freely jointed chains in **ID & 3 D);** influence of bond angle restriction, radius of gyration, thermodynamics of biopolymer solution (entropy of mixing & liquid state model along with limitation), free volume theory, heat and free energy of mixing.

IVth Semester

Paper XV CH-505 Physical Special-V 4 hrs. / Week
Max. Marks: 80
Time: 3 Hrs.

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Section-A

Statistical Thermodynamics:

Free energy functions and the partition functions, calculation of equilibrium constant using partition function, Bose - Einstein statistics, statistics of photon gas, gas degeneration, Fermi-Dirac statistics, extreme gas degeneration, energy of Bosons & Fermi particles, specific heat of electron gas, , Thermionic emission, comparison of Maxwell-Boltsmann, Bose –Einstein and Fermi-Dirac statistics.

Section-B

Non –Equilibrium Thermodynamics: General theory of non-equilibrium processes, entropy production and entropy flow; thermodynamic criteria for non-equilibrium states, entropy production in heat flow, mass flow, electric current, chemical reactions, Saxen's relation, Onsager's reciprocity relation, , Electro kinetic phenomenon.

Theory of fluctuation, energy fluctuations in the canonical ensemble, distribution function and fluctuations, fluctuations of density and energy.

Section-C

Angular Momentum : Angular momentum, angular momentum operators in cartesian coordinates, eigen function & eigen values, commutation relation between angular momentum operators (L_x,L_y , L_z , L^2), total orbital angular momentum and spin angular momentum, commutation relation between components of total orbital angular momentum and spin angular momentum, ladder operators, commutators of [L^2 , L_+] and [L^2 ,L_-] , application of ladder operators to an eigen function of L_z.

Section-D

Molecular Orbital Theory: Huckel molecular orbital (HMO) theory of llinear and cyclic conjugated systems, Applications of HMO theory to (i) set up and solve Huckel determent equation; (ii) calculate resonance energy; (iii) wave functions for molecular orbitals and molecular diagrams for the following :

(a) Ethylene molecule (b) Allyl system (Allyl radical and the related cation and anion) (c) Butadiene; (d) Cyclobutadiene (e) Cyclopropenyl system (cyclopropenyl radical and the related cation and anion

IVth Semester

Paper XVI CH-506 Physical Special-VI 4 hrs. / Week

Max. Marks: 80

Time: 3 Hrs.

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Section-A

Symmetry and Group Theory in Chemistry: Symmetry elements and symmetry operationgroup and its properties, Multiplication table, point symmetry groups. Schonflies symbol, representations of groups by matrices (representation for the C_n, C_{nv}, C_{nh}, D_{nh} etc. groups to be worked out explicity) Irreduceable representation of groups, the great orthogonality theorem (without proof) and its importance, character tables and their use in spectroscopy.

Section-B

Electronic Spectroscopy of Polyatomic Molecules : Free electron model, spectra of carbonyl group, spectra of ethene, n-II and II-II transitions, spectra of benzene , spectra of transition metals, charge-transfer transition, fluorescence phosphorescence.

Raman Spectroscopy : Quantum theory of Raman effect, Classical theory of Raman effect, Pure rotational Raman spectra, Raman activity of vibrations, vibrational Raman spectra, polarization of light and Raman effect, applications.

Section-C

Forms of Corrosion: Uniform corrosion, galvanic corrosion, pitting corrosion, crevice corrosion, intergranular corrosion, stress corrosion cracking, corrosion Dfatigue, fretting corrosion, dealloying, hydrogen embrittlement, erosion corrosion, microbial induced corrosion, filliform corrosion and exfoliation.

Section-D

Industrial Corrosion Problems: Atmospheric corrosion and high temperature oxidation. Corrosion in industrial cooling water system, corrosion in boilers and condensate pipe lines, corrosion due to acids, corrosion during metal surface cleaning and descaling, corrosion during storage and transportation of metallic articles, corrosion in various industries.

Paper-XVII CH-507 Physical Chemistry Practical

. (8Hrs. /Week)
Max. Marks: 80
Time: 8 Hrs

Potentiometry: Titrations

(i) NaOH vs. H_3PO_4 titration.

(ii) NaOH vs. (HCl + CH_3COOH) mixture

(iii) $K_2Cr_2O_7$ vs. Mohr's salt vs. $FeSO_4$

(iv) $AgNO_3$ vs. (KCl + KI) mixture

(v) Determination of solubility and solubility product of spairngly soluble salts($BaSO_4$) and AgCl.

(vi) Determination of degree of hydrolysis of aniline hydro chloride

(vii) Determination of dissociation constant of weak acid.

2. pH metry

Titrations

(i) NaOH vs. H_3PO_4

(ii) NaOH vs. (HCl + CH_3COOH) mixture

(iii) NH_4OH vs. HCl

(iv) NH_4OH vs. CH_3COOH

(v) Determination of composition of Copper amine complex from $CuSO_4$ vs. NH_4OH

(vi) Determination of dissociation constant of weak acid

(vii) Determination of dissociation constant of CH_3COOH in acetone by titrating it with KOH.

(viii) Determination of degree of hydrolysis of aniline hydro chloride.

3. Polarography

(i) Determination of half wave potential of Pb^{2+} , Cd^{2+} , CO^{2+}, Zn^{2+} , Mn^{2+} , Ni^{2+}

(ii) Estimation of cations in the given solution.

(iii) Ampereometry titration:- $Pb(NO_3)_2$ vs. $K_2Cr_2O_7$

4. Turbidimetry

(i) Determination of concentration of sulphate ions in the given solution.

Paper-XVIII CH-508 Physical Chemistry Practical

. (8Hrs. /Week)
Max. Marks: 80
Time: 8 Hrs

1. Conductometry Titrations:

(i) NaOH vs. oxalic acid
(ii) NaOH vs. (HCl + CH_3COOH) mixture
(iii) NaOH vs. (HCl + CH_3COOH + $CuSO_4$ mixture.
(iv) $AgNO_3$ vs. (KCl + KI) mixture
(v) Determination of concentration of Salicylic acid by
(a) Salt line method (b) Double alkali method
(vi) Determination of solubility and solubility product of sparingly soluble salt (Agcl, $Pbso_4$)
(vii) Determination of degree of hydrolysis and hydrolysis constant of analine hydro chloride in aqueous solution.
(viii) Study the kinetics of sponification of ester by NaOH conductometrically
(ix) Verification of D.H.O. equation for strong electrolytes.

2. Dipole metry

(i) To determine the dielectric constant of various liquids
(ii) To determine the dipole moment of a liquid

3. Polarimetry

(i) Determination of specific rotation for optically active substance
(ii) Estimation of concentration of optical active substance in the gtiven solution
(iii) Determination of percentage composition of optical substances in the given binary mixture (Glucose + Fructose or Tartaric acid)
(iv) Determination of rate constant for hydrolysis/inversion of sugar

4. Ultrasonic Interferrometry

(i) Determination of speed of sound for various liquids.

5. To determine the heat capacity of liquids and their mixtures

Paper-XIX CH-509 Physical Chemistry Practical

. (8Hrs. /Week)
Max. Marks: 140
Time: 8 Hrs

Spectrocolorimetry

(i) To test the validity of Lambert Beer's Law for $KMnO_4$ and $K_2Cr_2O_7$ in H_2SO_4

(ii) Determine the concentration of copper sulphate, potassium permanganate and potassium dichromate in their solution.

(iii) Determine the composition of the binary mixture containing $KMnO_4$ and $K_2Cr_2O_7$

2. Chemical Kinetics

(i) Saponification of ethyl acetate.

(ii) Determination of activation energy for the hydrolysis of ethyl acetate in presence of acid.

(iii) Relative strength of acids

(iv) Study of Iodination of acetone.

3. Flame Photometry

(i) To determine the concentration of Na^+ , Li^+ , Ca^{++} ions in the given solution

4. Viva -Voce: (30 Marks)

5. Practical Note Book (30 Marks)

IIIrd Semester

Paper XI **CH-501 Organic Special-I** 4 hrs. / Week

Max. Marks: 80

Time: 3 Hrs.

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Section-A

Ultraviolet and Visible Spectroscopy:

Introduction – Electronic energy levels, electronic transitions and selection rules. The origin, general appearance and designation of UV bands, absorption laws and measurement of absorption intensity, chromophores, auxochromes, bathochromic shift, hypsocromic shift, hypochromic effect, hyperchromic effect. The ultraviolet spectrometer-. Wood-ward and Fieser's rules for calculating ultraviolet absorption maxima for substituted dienes and conjugated dienes, unsaturated carbonyl compounds and aromatic carbonyl compounds. Application of UV spectroscopy to problems in organic chemistry.

Section-B

Infrared Spectroscopy:

Introduction – basic theory and instrumentation including FT IR infrared spectrum. Functional group and finger print regions. Absorption of infrared radiation and molecular vibrations. Fundamental vibrations and overtones. Intensity and position of infrared absorption bands, bands resulting from combination or difference of vibrational frequencies or by the interaction of overtones (or combination bands) with the fundamental vibrations (fermi resonance). Frequency of vibrations of a diatomic molecule, spectral features of major functional groups: alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols, ketones, aldehydes, esters, amides, acids, anhydrides, lactones, lactams, conjugated carbonyl compounds and amines. Effect of hydrogen bonding and solvent effect on vibrational frequencies, overtones, combination bands and fermi resonance. Applications of IR spectroscopy.

Section-C

Nuclear Magnetic Resonance Spectroscopy:

Introduction – spin active nuclei behave as spinning nuclear magnets, orientation of spinning nuclear magnets in a uniform magnetic field and energy description of NMR phenomenon, Continuous wave (CW) NMR spectrometer and Fourier transform (FT) NMR spectrometer. Phenomenon of resonance and relaxation, chemical shift , chemical shift parameters and internal standards, factors affecting the chemical shift: shielding and deshielding of a nucleus, substitution effects leading to empirical co-relations for proton chemical shifts, anisotropic effect, effect of changing solvents, effect of hydrogen bonding, influence of chirality on the chemical shifts of enantiomers and intermolecular Vander Walls deshielding, spin spin coupling, multiplicity of splitting and relative intensity of lines in a multiplet, integration, mechanism of coupling-one bond coupling (^{1}J), two bond coupling (^{2}J) three bond coupling (^{3}J) including Karplus relationship. Techniques for simplification of complex spectra: solvent effects, Lanthanide shift reagents, spin decoupling (double resonance), Fourier Transform technique, Nuclear Overhauser effect (NOE). Effect of sensitivity of C- 13 NMR compared to H–1 NMR, comparison of C–13 NMR and H-1NMR, chemical shifts of C–13 NMR. Simplification of C – 13 spectra by process of decoupling, off resonance decoupling.

Section-D

Mass Spectroscopy:

Introduction – basic theory , instrumentation, process of introducing the sample into mass spectrometer. Methods of generation of positively charged ions, electron ionization method , chemical ionization, FD and fast atom bombardment (FAB) techniques. Mass spectrum, base peak, molecular and parent ion, Mass to charge ratio (M/Z), relative intensity, fragment ions, even electron rule, nitrogen rule, matastable ions, McLafferty rearrangement and ortho effect. Determination of molecular weight and molecular formula using mass spectrometry

Optical Rotatory Dispersion (ORD) and Circular Dichroism (CD):

Defination, haloketo rule, octant rule for ketones.

Cotton effect and Cotton curves, deduction of absolute configuration.

IIIrd Semester

Paper XII CH-502 Organic Special-II 4 hrs. / Week

Max. Marks: 80

Time: 3 Hrs.

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Section-A

Vitamins

Structure and synthesis of vitamins A, B_1, B_2, B_6, C, D, E, nicotinic acid, pantothenic acid and Biotin

Section-B

Carotenoids:

General method of structure elucidation and synthesis of α-carotene, β-carotene, lycopene, γ-carotene. Biosynthesis of carotenoids

Porphyrins:

Structural , spectral properties and synthesis of porphyrins and Haemin. Structure of chlorophyll and Haemoglobin (without synthesis)

Section-C

Plant pigments:

Occurance, general chemical and spectroscopic methods for structure determination.

Structure elucidation and synthesis of Flavone, chrysin, Flavonol, Quercetin, Diadazin, Xanthone, Euxanthone, Cyanidin chloride, Malvidin chloride, Hirsudin chloride. Biosynthesis of flavonoids: Acetate pathway and shikimic acid pathways.

Section-D

Enzymes and co-enzymes:

Introduction to biological catalysis, nomenclature, classification and specificity.

Kind of reaction catalysed by enzymes: Oxidation – reduction, isomerisation, epimerisation, hydrolysis, phosphorylation, acylation, methylation, decarboxylation, dehydration.

Co-enzymes: Chemistry of Co-enzymes; Co-I, Co-II, Co-A, Co-carboxylase, FMN, FAD and Pyridoxal phosphate

IIIrd Semester

Paper XIII CH-503 Organic Special-II 4 hrs. / Week

Max. Marks: 80

Time: 3 Hrs.

Note:-*Examiner will set nine questions and the candidates will be required to attempt five questions in all. Out of nine questions one question will be compulsory containing eight short answer type questions covering the entire syllabus. Further examiner will set two questions from each section and the candidates will be required to attempt one question from each section. All questions will carry equal marks*

Section-A

Heterocyclic Compounds: General behaviour, Classification, Criteria of aromaticity, Tautomerism

Five membered Heterocycles: Synthesis and reactions of 1, 3-Azoles: Imidazole, Thiazole and Oxazole

Section-B

Six membered Heterocyclics with two heteroatoms: Detailed study of Pyrimidines and Purines.

Structural elucidation of uric acid and caffeine

Nucleosides and Nucleotides: Structure of Nucleosides and Nucleotides, General synthesis of Nucleotides and polynucleotides.

Section-C

Ylides:

General methods of formation, General study of reactions with their mechanisms of Nitrogen (Ammonium, Immonium, Diazonium and Nitrile), Phosphorous and Sulphur ylides and their applications.

Section-D

Synthetic Drugs:

Relation between physiological action and chemical constitution

Antimalarials, antipyretics, analgesics, sulphadrugs, Anthelmintics, antifertility, anticancer drugs.

IVrd Semester

Paper- XIV CH-504 Organic Special-IV

4 hrs. / Week
Max. Marks: 80
Time: 3 Hrs.

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Section-A

Photochemistry

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

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

Photochemistry of Carbonyl Compounds: Intramolecular reactions of carbonyl compounds, saturated, cyclic, acyclic, and α, β unsaturated compounds. Cyclohexadienones.

Section-B

Intermolecular cycloaddition reactions – dimerisations and oxetane formation.

Photochemistry of Aromatic Compounds: Isomerisations, additions and substitutions.

Miscellaneous Photochemical Reactions: Photo-Fries reactions of anilides. Photo-Fries rearrangement. Barton reaction. Singlet molecular oxygen reactions. Photodegradation of polymers.

Free Radicals: Free radicals stability, generation and detection. Types of free radical reactions, free radicals substation at an aromatic substrate, Hunsdiecker reaction.

Section-C

Pericyclic Reactions:

Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl system. Classification of pericyclic reactions. Woodward – Hoffmann correlation diagrams. FMO and PMO approach. Electrocyclic reactions – conrotatory and disrotatory motions, 4n, 4n+2 and allyl systems. Cycloadditions – antarafacial and suprafacial additions, 4n and 4n+2 systems, Sigmatropic rearrangements – suprafacial and antarafacial shifts of H, sigmatropic shifts involving carbon moieties, 3,3-and 5,5-sigmatropic rearrangements. Claisen,and Cope rearrangements

Section-D

Stereochemistry

Conformational analysis of medium and large membered rings, trans annular reactions, conformational analysis of cyclohexanone, effect of conformation on reactivity of acyclic and cyclic compounds.

Stereochemistry of nitrogen containing compounds, strain and their consequences in small ring heterocycles, conformation of six membered heterocyles. Barrier to ring inversion and pyramidal inversion and 1,3-diaxial interactions.

IVrd Semester

Paper- XV CH-505 Organic Special-V 4 hrs. / Week

Max. Marks: 80

Time: 3 Hrs.

Note:-*Examiner will set nine questions and the candidates will be required to attempt five questions in all. Out of nine questions one question will be compulsory containing eight short answer type questions covering the entire syllabus. Further examiner will set two questions from each section and the candidates will be required to attempt one question from each section. All questions will carry equal marks*

Section-A

Terpenoids:

Classification , nomenclature, occurrence and general method of structural determination , Isoprene rule, Stucture determination, stereochemistry and synthesis of Citral, Farnesol, Zingibrene, Santonin, α- Cadinene, Camphor and Abietic acid, Biogenetic pathways and biosynthesis

Section:- B

Alkaloids:

Classification, occurrence, general methods of isolation and structure elucidation. Structure, Stereochemistry , synthesis and biosynthesis of following : Papaverine, Nicotine, Quinine, morphine, lysergic acid and Reserpine

Section-C

Steroids and Harmons

Occurrence, General method of isolation, Diel's Hydrocarbon, Structure elucidation and synthesis of Cholesterol, Bile acids, Testosterone, Progesterone, Esterone and synthetic non-steroidal estrogens, oestrogens.

Structure elucidation and synthesis of Adrenaline and Thyroxine.

Section-D

Antibiotics

Structure elucidation of Pencillin, chloramphenicol, Streptomycin and Tetracyclins.

Prostaglandins:

Classification, Physiological effects and synthesis of PGE_2 and PGF2 α.

IVrd Semester

Paper- XVI CH-506 Organic Special-VI 4 hrs. / Week
Max. Marks: 80
Time: 3 Hrs.

Note:-*Examiner will set nine questions and the candidates will be required to attempt five questions in all. Out of nine questions one question will be compulsory containing eight short answer type questions covering the entire syllabus. Further examiner will set two questions from each section and the candidates will be required to attempt one question from each section. All questions will carry equal marks*

Section-A

Preparation, properties and applications of following reagents in organic synthesis with mechanistic details.

Organometallic Reagents:
n-Butyllithium, Grignard reagent, Organo chromium(III) compounds, Dialkyl copper lithium, Pentacarbonyl iron, Tetracarbonyl nickel, octacarbonyl, dicobalt, Alkene Palladium (II) complexes, Wilkinsons catalyst, Methyl triisopropoxy titanium, Tri-n-butyl tin hydride, Trimethyl silyl iodide, Diborane.

Section-B

General Reagents:
DCC I, 1,3-dithianes, Polyphosphoric acid, diazomethane, ethyldiazoacetate, Boron Trifluoride, Trifluoro acetic acid, cuprous chloride, N-bromosuccinamide,Mont- K-10, and KSF (clays). Phase Transfer catalysts.

Section-C

Oxidation:
Leadtetraacetate, osmium tetraoxide, selenium dioxide, potassium permanganate, Fenton's reagent, ozone, perbenzoic acid, periodic acid, chromium oxide, thallium (III) nitrate.

Reduction:
Catalytic hydrogenation, lithium aluminium hydride, sodium borohydride, sodamide, zinc dust, sodium liquid ammonia

Section-D

Rearrangements:
General mechanistic considerations – nature of migration, migratory aptitude,. A detailed study of following rearrangements. Pinacol – pinacolone, Wagner-Meerwein, Demjanov, Benzil-Benzilic acid, Favorskii, Arndt-Eistert synthesis, Neber, Beckmann, Hofman, Curtius, Schmidt, Baeyer-Villiger Shapiro reaction.

Paper-XIX CH-507 Organic Chemistry Practical

. (8Hrs. /Week)
Max. Marks: 80
Time: 8 Hrs

Multi-step Synthesis of Organic Compounds and Isolation of Organic Compounds from Natural Sources

(a) Multi-step synthesis: - **60 marks**

(i) Benzanilide from benzene
(ii) Benzilic acid from benzaldehyde
(iii) α-Acetylaminocinnamic acid from glycine
(iv) Acridone from anthranilic acid
(v) Meta - Nitroaniline from benzene
(vi) 5-Acetoxy-1,2-benzoxathiole-2 - one from hydroquinone
(vii) 2' - Hydroxy - 4 - methoxyphenyl styryl ketone from resorcinol
(Viii) p-nitrobenzanilide from Benzophenone

(b) Isolation **20 marks**

(i) Caffeine from tea leaves
(ii) Lactose and casein from milk
(iii) Cystine from human hair
(iv) D (+)Glucose from cane sugar
(v) Hippuric acid from urine

Paper-XIX CH-508 Organic Chemistry Practical

. (8Hrs./Week)
Max. Marks: 80
Time: 8 Hrs

Qualtitative Analysis

Identification of organic compounds using spectroscopic methods (IR, UV, NMR & Mass) followed by characterization by chemical methods.

Note: Two sets to be given in the examination

(2×40 Marks)

Paper-XIX CH-509 Organic Chemistry Practical

. (8Hrs./Week)
Max. Marks: 140
Time: 8 Hrs

Quantitative Analysis (50 Marks)

(a) Determination of percentage or number of hydroxyl groups in organic compound by acetylation method.

(b) Estimation of Amines/ phenols using bromate - bromide solution/or acetylation method.

(c) Determination of iodine and saponification values of oil samples.

(d) Determination of concentration of Glucose / or Sucrose in the given solution

2. Spectrophotometric (UV/VIS) Estimations :

(30 Marks)

(a) Amino acids

(b) Proteins

(c) Carbohydrates

(d) Ascorbic acid

(e) Aspirin

(f) Caffeine

(g) Cholesterol

3. Viva-Voce (30 Marks)

4. Note Book (30Marks)