

Maharaja Ganga Singh University, Bikaner (Raj)
M.Sc. Chemistry Semester Scheme 2024-25

M.Sc. Chemistry : Program Structure and Examination scheme

Semester I

| Course Code | Name of the course | Max Marks (Passing Marks) | External M.M. (Passing Marks) | Internal M.M. (Passing Marks) |
|--------------------|-------------------------------|--------------------------------------|--|--|
| CC-1 | Inorganic Chemistry-1 | 50 (13) | 40 (10) | 10 (3) |
| CC-2 | Organic Chemistry-1 | 50 (13) | 40 (10) | 10 (3) |
| CC-3 | Physical Chemistry-1 | 50 (13) | 40 (10) | 10 (3) |
| CC-4 | Analytical Chemistry-1 | 50 (13) | 40 (10) | 10 (3) |
| LC-1 | Lab-1 | 50 (18) | 40 (14) | 10 (4) |
| LC-2 | Lab-2 | 50 (18) | 40 (14) | 10 (5) |
| | | 300 (108) | 240 (86) | 60 (22) |

- Aggregate Passing marks are 36% i.e. 108 in each semester whereas in each paper passing marks are 25%. In Lab course passing marks are 36%.
- Each theory paper will be of 4h per week and lab work (practical) 24hrs per week (each lab of 12 h).
- Internal examination will be conducted at Institution level as per instructions and a proper record will be maintained for it, which should be posted to MGSU within a specified time.
- A board of two examiners will be formed at the Institution level for Internal Practical exams.
- A board of three examiners will be formed (at least one external examiner should be in board) for the conduction of external examination of practical. The external practical examination should be conducted in 14 hrs spreaded in two days.
- For Internal laboratory work (Practical) in each semester – Seminar and project / survey / tour should be conducted and should be considered during evaluation. The project / survey should be based on local problems and or local industry needs etc.
- There will be three sections in each theory paper Section A – 10 questions each carrying 1 mark (two questions from each unit), Section B – 5 question (two questions from each unit with an internal choice of attempting one) each carrying 3 marks, Section C - five question (one from each unit and three questions are to be attempted) each carrying 5 marks.

Scheme for External Examination : Marks distribution for Lab1

- Practical 1 (select one from A) -10 marks
- Practical 2 (select one from B) -10 marks
- Practical 3 (select one from C) -10 marks
- Spotting (select 5 spots) -5 marks
- Viva and Record – 2+3 -5 marks

Scheme for External Examination : Marks distribution for Lab2

- Practical 1 (select one from A) -10 marks
- Practical 2 (select one from B) -10 marks
- Practical 3 (select one from C) -10 marks
- Project and Seminar -5 marks
- Viva and Record – 2+3 -5 marks

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Semester II

| Course Code | Name of the course | Max Marks (Passing Marks) | External M.M. (Passing Marks) | Internal M.M. (Passing Marks) |
|--------------------|-------------------------------|--------------------------------------|--|--|
| CC-5 | Inorganic Chemistry-2 | 50 (13) | 40 (10) | 10 (3) |
| CC-6 | Organic Chemistry-2 | 50 (13) | 40 (10) | 10 (3) |
| CC-7 | Physical Chemistry-2 | 50 (13) | 40 (10) | 10 (3) |
| CC-8 | Analytical Chemistry-2 | 50 (13) | 40 (10) | 10 (3) |
| LC-3 | Lab-3 | 50 (18) | 40 (14) | 10 (4) |
| LC-4 | Lab-4 | 50 (18) | 40 (14) | 10 (5) |
| | | 300 (108) | 240 (86) | 60 (22) |

- Aggregate Passing marks are 36% i.e. 108 in each semester whereas in each paper passing marks are 25%. In Lab course passing marks are 36%.
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- Internal examination will be conducted at Institution level as per instructions and a proper record will be maintained for it, which should be posted to MGSU within a specified time.
- A board of two examiners will be formed at the Institution level for Internal Practical exams.
- A board of three examiners will be formed (at least one external examiner should be in board) for the conduction of external examination of practical. The external practical examination should be conducted in 14 hrs spreaded in two days.
- For Internal laboratory work (Practical) in each semester – Seminar and project / survey / tour should be conducted and should be considered during evaluation. The project / survey should be based on local problems and or local industry needs etc.
- There will be three sections in each theory paper Section A – 10 questions each carrying 1 mark (two questions from each unit), Section B – 5 question (two questions from each unit with an internal choice of attempting one) each carrying 3 marks, Section C - five question (one from each unit and three questions are to be attempted) each carrying 5 marks.

Scheme for External Examination : Marks distribution for Lab 3

- Practical 1 (select one from A) -10 marks
- Practical 2 (select one from B) -10 marks
- Practical 3 (select one from C) -10 marks
- Spotting (select 5 spots) -5 marks
- Viva and Record – 2+3 -5 marks

Scheme for External Examination : Marks distribution for Lab 4

- Practical 1 (select one from A) -10 marks
- Practical 2 (select one from B) -10 marks
- Practical 3 (select one from C) -10 marks
- Project and Seminar -5 marks
- Viva and Record – 2+3 -5 marks

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Semester III

| Course Code | Name of the course | Max Marks (Passing Marks) | External M.M. (Passing Marks) | Internal M.M. (Passing Marks) |
|---|--|------------------------------|----------------------------------|----------------------------------|
| CC-9 | Spectral techniques and applications | 50 (13) | 40 (10) | 10 (3) |
| CC-10 | Introduction to recent advances in chemical sciences | 50 (13) | 40 (10) | 10 (3) |
| CC-11- (choose only one from A/B/C/D) | A Specialization I – Inorganic Chemistry - Advanced Inorganic Chemistry Pt1 B Specialization II – Organic Chemistry - Organic Synthesis Pt1 C Specialization III – Physical Chemistry Recent Trends in Physical Chemistry Pt1 (physical-organic chemistry) D Specialization IV – Analytical Chemistry - Analytical chemistry Pt1 | 50 (13) | 40 (10) | 10 (3) |
| CC-12-- (choose only one from A/B/C/D) | A Specialization I – Inorganic Chemistry - Metal Complexes and Polymers B Specialization II – Organic Chemistry - Heterocyclics and Natural Products Pt1 C Specialization III – Physical Chemistry Advances in electrochemistry D Specialization IV – Analytical Chemistry Applied Analytical Chemistry Pt1 | 50 (13) | 40 (10) | 10 (3) |

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| | | | | |
|---|---------------------------|---------------------|--------------------|-------------------|
| LC-5 (choose only one from A/B/C/D) | Lab-5 (A/B/C/D) | 50 (18) | 40 (14) | 10 (4) |
| LC-6 (choose only one from A/B/C/D) | Lab-6 (A/B/C/D) | 50 (18) | 40 (14) | 10 (5) |
| | | 300 (108) | 240 (86) | 60 (22) |

- Aggregate Passing marks are 36% i.e. 108 in each semester whereas in each paper passing marks are 25%. In Lab course passing marks are 36%.
- For CC-11, 12 and LC-5,6 students are allowed to select a group i.e. A/B/C/D
- Each theory paper will be of 4h per week and lab work (practicals) 24hrs per week (each lab of 12 h).
- Internal examination will be conducted at Institution level as per instructions and a proper record will be maintained for it, which should be posted to MGSU within a specified time.
- A board of two examiners will be formed at the Institution level for Internal Practical exams.
- A board of three examiners will be formed (at least one external examiner should be in board) for the conduction of external examination of practical, The examination should be conducted in 14 hrs spreaded in two days.
- For Internal laboratory work (Practical) in each semester – Seminar and project / survey / tour should be conducted and should be considered during evaluation. The project / survey should be based on local problems and or local industry needs etc.
- There will be three sections in each theory paper Section A – 10 questions each carrying 1 mark (two questions from each unit), Section B – 5 question (two questions from each unit with an internal choice of attempting one) each carrying 3 marks, Section C - five question (one from each unit and three questions are to be attempted) each carrying 5 marks.

Scheme for External Examination : Marks distribution for Lab 5

- Practical 1 (select one from A) -10 marks
- Practical 2 (select one from B) -10 marks
- Practical 3 (select one from C) -10 marks
- Spotting (select 5 spots) -5 marks

- Viva and Record – 2+3 -5 marks

Scheme for External Examination : Marks distribution for Lab 6

- Practical 1 (select one from A) -10 marks
- Practical 2 (select one from B) -10 marks
- Practical 3 (select one from C) -10 marks
- Project and Seminar -5 marks
- Viva and Record – 2+3 -5 marks

M.Sc. Chemistry : Program Structure and Examination scheme

Semester IV

| Course Code | Name of the course | Max Marks (Passing Marks) | External M.M. (Passing Marks) | Internal M.M. (Passing Marks) |
|---|--|--------------------------------------|--|--|
| CC-13 | Advances in spectroscopy and photo chemistry | 50 (13) | 40 (10) | 10 (3) |
| CC-14 | Chemical biology and computer in chemistry | 50 (13) | 40 (10) | 10 (3) |
| CC-15- (choose only one from A/B/C/D) | <p>A Specialization I – Inorganic Chemistry</p> <p>- Advanced Inorganic Chemistry Pt 2</p> <p>B Specialization II – Organic Chemistry</p> <p>- Organic Synthesis Pt 2</p> <p>C Specialization III – Physical Chemistry</p> <p>- Recent Trends in Physical Chemistry</p> <p>D Specialization IV – Analytical Chemistry</p> <p>- Analytical chemistry Pt 2</p> | 50 (13) | 40 (10) | 10 (3) |
| CC-16-- (choose only one from A/B/C/D) | <p>A Specialization I – Inorganic Chemistry</p> <p>- Ceramics and Advanced Polymers</p> <p>B Specialization II – Organic Chemistry</p> <p>- Heterocyclics and Natural Products Pt2</p> <p>C Specialization III – Physical Chemistry</p> <p>- Computational Chemistry</p> <p>D Specialization IV – Analytical Chemistry</p> | 50 (13) | 40 (10) | 10 (3) |

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| | Applied Analytical Chemistry Pt2 | | | |
|---|----------------------------------|---------------------|--------------------|-------------------|
| LC-7 (choose only one from A/B/C/D) | Lab-7 (A/B/C/D) | 50 (18) | 40 (14) | 10 (4) |
| LC-8 (choose only one from A/B/C/D) | Lab-8 (A/B/C/D) | 50 (18) | 40 (14) | 10 (5) |
| | | 300 (108) | 240 (86) | 60 (22) |

- Aggregate Passing marks are 36% i.e. 108 in each semester whereas in each paper passing marks are 25%. In Lab course passing marks are 36%.
- For CC-15, 16 and LC-7,8 students are allowed to select a group i.e. A/B/C/D
- Each theory paper will be of 4h per week and lab work (practical) 24hrs per week (each lab of 12 h).
- Internal examination will be conducted at institution level as per instructions and a proper record will be maintained for it, which should be posted to MGSU within a specified time.
- A board of two examiners will be formed at the institution level for Internal Practical exams.
- A board of three examiners will be formed (at least one external examiner should be in board) for the conduction of external examination of practical, The examination should be conducted in 14 hrs spreaded in two days.
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- There will be three sections in each theory paper Section A – 10 questions each carrying 1 mark (two questions from each unit), Section B – 5 question (two questions from each unit with an internal choice of attempting one) each carrying 3 marks, Section C - five question (one from each unit and three questions are to be attempted) each carrying 5 marks.

Scheme for External Examination : Marks distribution for Lab 7

- Practical 1 (select one from A) -10 marks
- Practical 2 (select one from B) -10 marks
- Practical 3 (select one from C) -10 marks

- Spotting (select 5 spots) -5 marks
- Viva and Record – 2+3 -5 marks

Scheme for External Examination : Marks distribution for Lab 8

- Practical 1 (select one from A) - 4 marks
- Practical 2 (select one from B) -4 marks
- Practical 3 (select one from C) - 4 marks
- Spotting - 4 marks
- Seminar (on selected topic) – 4 marks
- Project and Presentation - 20 marks

Semester 1

PAPER-I CC-1

INORGANIC CHEMISTRY - 1

Time : 3 Hours

Max. Marks :50 (40 for external 10 for internal)

Unit-I

Stereochemistry and Bonding in main group compounds : VSEPR, Walsh diagrams (Tri and penta- atomic molecules), $d\pi$ - $p\pi$ bonds, Bent rule and energetic of hybridization, some simple reactions of covalently bonded molecules: atomic inversion and Berry pseudorotation.

Unit-II

Reaction Mechanism of Transition Metal Complexes (Part 1): Energy profile of a reaction, reactivity of metal complexes, inert and labile complexes, kinetic application of valence bond and crystal field theories kinetics of octahedral substitution, acid hydrolysis, factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism, direct and indirect evidences in favour of conjugate mechanism, anation reactions, reactions without metal ligand bond cleavage.

Unit-III

Reaction Mechanism of Transition Metal Complexes (Part 2): Substitution reactions in square planar complexes, the trans effect, mechanism of the substitution reactions. Redox reactions, electron transfer reactions, mechanism of one electron transfer reactions, outer sphere type reactions, cross reactions and Marcus Hush theory, inner sphere type reactions.

Unit-IV

Metal - Ligand Bonding : Limitations of Crystal field theory, molecular orbital theory: octahedral, tetrahedral and square planar complexes, π - bonding and molecular orbital theory, explanation of position of the ligands in Spectrochemical series using MOT and Comparison with CFT.

Unit-V

Green chemistry Principles and applications in synthesis and analysis. Safety rules and safe use of different materials and chemical and biochemical weapons.

Books Suggested :

- 1- Advanced inorganic Chemistry, F.A. Cotton and Wilkinson, John Wiley.
- 2- Inorganic Chemistry, J.E. Huhey, Harpers & Row.
- 3- Chemistry of the elements, N.N. Greenwood and A. Earnsho, Pergamon.
- 4- Inorganic Electronic Spectroscopy, A.B.P. Lever, Elsevier.
- 5- Magneto chemistry, R.L. Carlin, Springer Verlag.
- 6- Comprehensive Coordination Chemistry eds. G. Wilkineson, R.D. Gillars and J.A. McCleverty, Pergamon.

- 7- Green Chemistry Theory and Practice, Paul T. Anastas and John C. Warner, Oxford University Press.

PAPER-II CC-2
ORGANIC CHEMISTRY -1

Time : 3 Hours

Max. Marks :50 (40 for external 10 for internal)

Unit-I

Nature of Bonding in organic Molecules : Delocalized chemical bonding—conjugation, cross conjugation, resonance, hyperconjugation, bonding influence tautomerism.

Aromaticity in benzenoid and non- benzenoid compounds alternant and non alternant hydrocarbons, Huckel's rule, energy level of molecular orbital, annulenes, anti aromaticity, Psi aromaticity homo aromaticity. PMO approach. Bonds weaker than covalent- addition compounds, crown ether complexes and cryptands, inclusion compounds cyclodextrins, catenane and rotaxanes.

Unit-II

Reaction Mechanism : Structure and Reactivity : Type of mechanisms, types of reaction, thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammonds'Postulates,curtin Hammett Principle Potential energy Diagrams, transition states and intermediates, methods of determining mechanisms, isotope effects. Hard and soft acids and bases. Generation, structure stability and reactivity of carbocations, carbanions, free radical, carbenes and nitrenes. Effect of structure on reactivity of carbocations, carbanions, free radicals, carbenes and nitrenes. Effect of structure on reactivity- resonance and field effects, steric effect, quantitative treatment. The hammett equation and linear free energy relationship, substituent and reaction constants. Taft equation.

Unit-III

(a) Aliphatic Electrophilic Bimolecular mechanism SE^1 and SE^2 the SE mixed mechanism, electrophilic substitution accompanied by double bond shifts. Effect of substrates, leaving group and the solvent polarity on the reactivity.

(b) **Aromatic Electrophilic Substitution :** The arenium ion mechanism, orientation and reactivity, energy profile diagrams. The ortho/ para ratio, ipso attack, orientation in other ring systems. Quantitative treatment of reactivity in substrates and electrophiles. Diazonium coupling. Vilsmeier reaction, Gattermann-Koch reaction.

Unit-IV

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.

Unit-IV

Elimination Reactions : The E_2 , E_1 and E_{1cb} mechanisms and their spectrum. Orientation of the double bond, reactivity effects of substrate structures, attacking base, the leaving groups and the medium. Mechanism & orientation in pyrolytic elimination.

Books Suggested :

- 1- Advanced Organic Chemistry – Reactions, Mechanism and Structure, Jerry March, John Wiley.
- 2- Advanced Organic Chemistry, F.A. Carey and R.J. Sundberg. Plenum.
- 3- A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman.
- 4- Structure and Mechanism in Organic Chemistry, C.K. Ingold, Cornell University Press.
- 5- Organic chemistry, R.T. Morrison and R.N. Boyd, Prentice Hall.
- 6- Modern Organic synthesis, R.O.C. Norman and J.M. Coxon Blackie Academic & Professional.
- 7- Principles of Organic Synthesis, R.O.C. Norman and J.M. Coxon, Blackie Academic & Professional.
- 8- Pericyclic Reactions, S.M. Mukherji, Macmillan India.
- 9- Reaction Mechanism in Organic Chemistry, S.M. Mukherji and S.P. Singh Macmillan.
- 10- Stereochemistry of Organic Compounds. P.S. Kalasi, New Age International.

PAPER-III CC- 3

PHYSICAL CHEMISTRY - 1

Time : 3 Hours

Max. Marks :50 (40 for external 10 for internal)

Unit-I

Quantum Chemistry

(a) Introduction to Exact Quantum Mechanical Results : The Schrödinger equation and the postulates of quantum mechanics. Discussion of solutions of the Schrödinger equation to some model systems viz., particle in a box, the harmonic oscillator, the rigid rotator, the hydrogen atom.

(b) Approximate Methods : The variations theorem, linear variation principle. Perturbation theory (first order and non-degenerate). Application of variation methods and perturbation theory to the Helium atoms.

Unit-II

Thermodynamics Part 1

(a) Classical Thermodynamics : Brief resume of concepts of laws of thermodynamics, free energy 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 coefficient, ionic strength. Application of phase rule to three component systems; second order phases transitions.

Unit-III

Chemical Dynamics :

Methods of determining rate laws, collision theory of reaction rates, steric factor, activated complex theory, arrhenius equation and the activated complex theory, ionic reactions, kinetic salt effects, steady state kinetics, kinetic and thermodynamic control of reactions, treatment of unimolecular reactions.

Unit-IV

Chemical Dynamics :

Dynamic chain (hydrogen-bromine reaction, pyrolysis of acetaldehyde, decomposition of ethane), photochemical (hydrogen –bromine and hydrogen chlorine reactions) and oscillatory reactions (Belousov-zhabotinsky reaction), homogeneous catalysis, kinetics of enzyme reactions, general features of Fast reactions, study of fast reactions by flow method, relaxation method, flash photolysis and the nuclear magnetic resonance method. Dynamics of molecular motions, probing the transition state, dynamics of barrier less chemical reactions in solution, dynamics of unimolecular reactions (Linde-mann-Hinshelwood and Rice- Ramsperger-Kassel-Marcus [RRKM] theories of unimolecular reactions).

Unit- V

Surface Chemistry

(a) Adsorption : Surface tension, capillary action, pressure difference: across curved surface (laplac-equation), vapour pressure of droplets (Kelvin equation) , Gibbs adsorption , isotherm , estimation of surface area (BET equation), Surface films on liquids (Electro-kinetic phenomenon) Catalytic activity at surfaces.

(b) Micelles : Surface active agents, classification of surface active agents, micellization, hydrophobic interaction, critical micellar concentration (CMC) , factors affecting the CMC of surfactants, counter ion binding to micelles, thermodynamics of micellization-phase separation and mass action models , solubilization, micro emulsion, reverse micelles.

Books 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 Kinetics, K.J. Laidler, McGraw Hill.
6. Kinetics and Mechanism of Chemical Transformations, J. Rajaraman and J. Kuriacose, McMillan.
7. Micelles, Theoretical and Applied Aspects, V. Moroi, Plenum.

8. Modern Electrochemistry Vol. 4 and Vol. II, J.O.M. Bockris and A.K.N. Reddy,. Plenum.
9. Introduction to Polymer Science, V.R. Gowarikar, N.V. Vishwanathan and J. Sridhar, Wiley Easter.

Paper-IV : CC-4

ANALYTICAL CHEMISTRY -1

Time : 3 Hours

Max. Marks :50 (40 for external 10 for internal)

Unit-I

Drug analysis - Principles of determination of functional groups ; Protocols for the analysis of standard drugs. Food standards and Specifications Anti microbial agents / Class I and Class II preservatives as per PFA Act.

Unit II

Electroanalytical Methods:

Potentiometry/ pH- metry: Basic principles, instrumentation, experimental technique, electrodes-reference, indicate-ion sensitive and recent advances in potentiometry and application.

Conductometry: Basic Principle, instrumentation, experimental technique, Low & High frequency titration.

Unit-III

Atomic Spectroscopy : Energies of atomic orbitals, vector representation of momenta and vector coupling, spectra of hydrogen atom and alkali metal atoms.

Molecular Spectroscopy : Energy levels, molecular orbitals, vibronic transitions, vibrational progressions and geometry of the excited states, Franck-Condon principle, electronic spectra of polyatomic molecules. Emission spectra; radiative and non-radiative decay, internal conversion.

Unit-IV

Theory Principle, instrumentation, experimental techniques and application of IR, FTIR, Raman, Laser Raman and Uv-vis spectroscopy.

Unit-V

X-Ray Diffraction : Bragg condition, Miller indices, Laue methods, Bragg method Debye Scherrer method of X-ray structural analysis of crystal, index reflections, identification of unit cells 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, Ramchandran diagram.

Books Suggested:

1. Modern Spectroscopy, J.M. John Wiley.

2. Applied Electron Spectroscopy for Chemical Analysis Ed. H. Windawi and F.L Ho, Wiley Interscience.
3. NMR, NQR, EPR and Mossbaur Spectroscopy in Inorganic Chemistry, R.V. Parish, Ellis Harwood.
4. Physical Methods in Chemistry, R.S. Drago, Saunders College.
5. Chemical Applications of Group Theory, FA. Cotton.
6. Introduction to Molecular Spectroscopy, R. Chang, McGraw Hill.
7. Basic Principles of Spectroscopy, R. Chang, McGraw Hill.
8. Theory and Applications of UV Spectroscopy, H.H. Jaffeand M. Orchin,
9. Introduction to Photoelectron Spectroscopy, P.K; Ghosh, John Wiley.
10. Introduction to Magnetic Resonance, A. Carrington and A.D. Carrington and AD. Maclachalan, Harper & Row.

M.Sc. CHEMISTRY PRACTICAL

LC-1

Lab 1

Time : 7 Hours

Max. Marks :50 (40 for external 10 for internal)

A.

Safety in laboratory - Identification of safety symbols, Safety in Laboratory, Chemical hazards and safety parameters in laboratory, industry and daily life. Ethics and behavior in laboratory. Types and Working of fire extinguishers. MSDS study and preparation.

B.

Qualitative Analysis -

- (a) Analysis of Inorganic mixture containing eight radicals, out of which at least one should be less common metal ion
- (b) Insoluble-oxides, sulphates and halides. Interfering radicals

Preparations

Preparations of selected inorganic compounds and their studies by I.R., electronic spectra, Mossbauer, E.S.R and magnetic susceptibility measurements. Handling of air and moisture sensitive compounds. Study of instruments related to various techniques described in syllabus.

- | | |
|--|--|
| (1) VO (acac) | (2) TiO (C ₉ H ₈ NO) 2H ₂ O |
| (3) cis-K [Cr (C ₂ OH) ₂ (H ₂ O) ₂] | (4) Na[Cr(NH ₃) ₂ (SCN) ₄] |
| (5) Mn(acac) ₃ | (6) K ₂ [Fe(C ₂ O ₄) ₃] |
| (7) Prussian blue, Turnbull's Blue | (8) [CO(NH ₃) ₆][Co(NO ₂) ₆] |

C.

Virtual Chemistry Experiments

Experiments related with molecular modeling, virtual synthesis, virtual titrations, virtual chromatography etc. can be performed.

Phase Equilibria

- (i) Determination of congruent composition and temperature of a binary system (e.g.) diphenylamine-benzophenone system)
- (ii) Determination of transition temperature of a given salt(e.g., CaCl_2) conductometrically.
- (iii) To construct the phase diagram for three component system (e.g.) chloroform -acetic acid-water).

Spotting

IKS : Primary information on experimental methods in Indian Knowledge system (chemical science)

M.Sc. CHEMISTRY PRACTICAL

LC-2

Lab 2

Time : 7 Hours

Max. Marks :50 (40 for external 10 for internal)

A. Organic chemistry

Qualitative Analysis

Separation, purification and identification of compounds of binary mixture (one liquid and one solid) using TLC and column chromatography, chemical tests. IR spectra to be used for functional group identification.

Organic Synthesis (Any Five)

- 1- Acetylation : Acetylation of cholesterol and separation of cholesteryl acetate by column chromatography.
- 2- Oxidation : Adipic acid by chromic acid oxidation of cyclohexanol.
- 3- Grignard reaction : synthesis of triphenyl methanol from benzoic acid.
- 4- Aldol condensation : Dibenzal acetone from benzaldehyde.
- 5- Sandmeyer reaction : p chlorotoluene from p-toluidine.

B. Physical Chemistry

Adsorption –

To Study surface tension-concentration relationship for solutions (Gibb's equations)

Chemical Kinetics :

- (i) Determination of the effect (a) Change of temperature (b) Change of concentration of reactants and catalyst and (c) Ionic strength of the media on the velocity constant of hydrolysis of an ester / ionic reactions.
- (ii) Determination of the velocity constant of hydrolysis of an ester / ionic reaction in micellar media.

- (iii) Determination of the rate constant for the oxidation of iodide ions by hydrogen peroxide studying the kinetics as iodine clock reaction.
- (iv) Flowing clock reactions (Ref. :Experiments in Physical chemistry by Showmaker).
- (v) Determination of the primary salt effect on the kinetics of ionic reactions and testing of the Bronsted relationship (iodide ion is oxidized by persulphate ion)
- (iv) Oscillatory reaction.

C.

Analytical Chemistry - Error Analysis and Statistical Data Analysis:

Experiments based on Errors, type of errors, minimization of errors, error distribution curves, precision, accuracy and combination, statistical treatment for error analysis, student 'T' test null hypothesis, rejection criteria F & Q test; linear regression analysis, curve fittings,.

Calibration of volumetric apparatus, burette, pipette, standard flask etc.

Spotting

IKS : Primary information on experimental methods in Indian Knowledge system (chemical science)

Reference Books:

- 1- Vogel's Textbook of Quantitative Analysis, revised, J. Bassett, R.C. Denney, G.H. Jeffrey and J. Mendham, ELBS.
- 2- Experiments and Techniques in Organic Chemistry, D.P. Pasto, C Johnson and M. Miller, Prentice Hall.
- 3- Macroscale and Microscale Organic Experiments, K.L. Williamson D.C. Heath.
- 4- Systematic Qualitative Organic Analysis, H. Middleton, Edward Arnold.
- 5- Vogel's Textbook of Practical Organic Chemistry, A.R. Tatchell,
- 6- Practical Physical chemistry, A.M. James and F.E. Porichard, Longman.
- 7- Findley's Practical Physical Chemistry, B.P. Levitt, Longman.
- 8- Experimental Physical Chemistry R.C. Das and B. Behera,
- 9- Green Chemistry : An experimental study, R.K. Sharma, N. Bhojak, I.T. Sidhwani and M.K. Choudhary

Semester 2

PAPER-I CC-5

INORGANIC CHEMISTRY – 2

Time : 3 Hours

Max. Marks :50 (40 for external 10 for internal)

Unit-I

Metal-Ligand Equilibria in Solution : Stepwise and overall formation constants and their interaction, trends in stepwise constant, factors affecting the stability of metal complexes with reference to the nature of metal ion and ligand, chelate effect and its thermodynamic origin, determination of binary formation constants by pH-metry and spectrophotometry.

Unit-II

Electronic spectra and magnetic properties of transition metal complexes spectroscopic ground states, correlation, Orgel and Tanabe-sugano diagram for transition metal complexes (d^1 - d^9 - states) calculations of Dq , B and b parameters, charge transfer spectra spectroscopic method of assignment of absolute configuration in optically active metal chelates and their chemical information, magnetic moments magnetic exchange coupling and spin crossover.

Unit-III

Symmetry and Group theory in chemistry- symmetry elements and symmetry operation, definition of group sub group, relation between orders of a finite group and subgroup conjugacy relation and classes. Point symmetry group Schoenflies symbols representation of groups by matrices. Character of a representation. The great orthogonality theorem and its importance Character tables and their use.

Unit-IV

Metal p Complexes : Metal carbonyls, structure and bonding, vibration spectra of metal carbonyls for bonding and structural elucidation, important reactions of metal carbonyls; preparation, bonding, structure and important reactions of transition metal nitrosyl, dinitrogen and deoxygenate complexes; tertiary phosphine as ligand.

Unit-V

Metal Clusters : Higher boranes, carboranes, metalloboranes and metallocarboranes. Metal carbonyl and halide clusters, compounds with metal-metal multiple bonds.

Magnetic Properties of Transition Metal Complexes: Anomalous magnetic moments, magnetic exchange coupling and spin crossover.

ORD and CD: Introduction, assignment of absolute configuration in optically active metal chelates and their configuration.

Books Suggested :

- 1- Advanced inorganic Chemistry, F.A. Cotton and Wilkinson, John Wiley.

- 2- Inorganic Chemistry, J.E. Huhey, Harpers & Row.
- 3- Chemistry of the elements, N.N. Greenwood and A. Earnsho, Pergamon.
- 4- Inorganic Electronic Spectroscopy, A.B.P. Lever, Elsevier.
- 5- Magneto chemistry, R.L. Carlin, Springer Verlag.
- 6- Comprehensive Coordination Chemistry eds. G. Wilkineson, R.D. Gillars and J.A. McCleverty,
7. F. Basolo and R.G. Pearson: Mechanism of Inorganic Reaction, Wiley Eastern.

PAPER-II CC-6
ORGANIC CHEMISTRY -2

Time : 3 Hours

Max. Marks :50 (40 for external 10 for internal)

Unit-I

Stereochemistry : Conformational analysis of cycloalkanes, decaline, effect of conformation on reactivity, conformation of sugars, steric strain due to unavoidable crowding. Elements of symmetry, chirality, molecules with more than one chiral center, threo and erythro isomers method of resolution, optical purity enantiotropic and diastereotopic atoms, groups and faces, stereospecific and stereo selective synthesis. Asymmetric synthesis. Optical activity in the absenece of chiral carbon (biphenyls, allenes and spiranes), chirality due to Helical Shape.

Stereochemistry of the compounds containing nitrogen, sulphur and phosphours.

Unit-II

Aliphatic Nucleophilic Substitution : The SN^1 , SN^2 , mixed SN^1 and SN^2 and SET mechanisms, neighbouring group participation by Sigma and Pie bonds. Anchimeric assistance. Classical and nonclassical carbocations, phenonium ions norbornyl system, common carbocations rearrangements. Application of NMR spectroscopy in the detection of carbocations. The SN mechanisms. Nucleophilic substitution at an allylic, aliphatic trigonal and a vinylic carbon reactivity effects of substrate structure attacking nucleophile, leaving group and reaction medium, phase transfer catalysis and ultrasound, ambidentate nucleophile, regioselectivity.

Unit-III

(a) Aromatic Nucleophilic substitution : the $SN Ar$, SN , Benzyne and SRN mechanisms. Reactivity-effect of substrate structure, leaving group and attacking nucleophile. The Von richter, sommelet- Hauser and Smiles rearrangements.

(b) Free Radical Reactions : Types of free radical reactions, free radical substitution mechanisms, mechanism at an aromatic substrate, neighbouring group assistance, Reactivity for aliphatic and aromatic substrates at a bridgehead. 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

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

Unit-V

Pericyclic Reactions : Molecular orbital symmetry, frontier orbital 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, $2+2$ addition of ketenes, 1,3 dipolar cycloadditions and cheletropic reactions. Sigmatropic rearrangements – suprafacial and antarafacial shifts of H sigmatropic shifts involving carbon moieties, 3,3, - and 5,5- sigmatropic rearrangements. Claisen, Cope and aza-cope rearrangements. Fluxional tautomerism. Ene reaction.

Books Suggested :

- 1- Advanced Organic Chemistry – Reactions, Mechanism and Structure, Jerry March, John Wiley.
- 2- Advanced Organic Chemistry, F.A. Carey and R.J. Sundberg. Plenum.
- 3- A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman.
- 4- Structure and Mechanism in Organic Chemistry, C.K. Ingold, Cornell University Press.
- 5- Organic chemistry, R.T. Morrison and R.N. Boyd, Prentice Hall.
- 6- Modern Organic synthesis, R.O.C. Norman and J.M. Coxon Blackie Academic & Professional.
- 7- Principles of Organic Synthesis, R.O.C. Norman and J.M. Coxon, Blackie Academic & Professional.
- 8- Pericyclic Reactions, S.M. Mukherji, Macmillan India.
- 9- Reactions Mechanism in Organic Chemistry, S.M. Mukherji and S.P. Singh Macmillan.
- 10- Stereochemistry of Organic Compounds. P.S. Kalasi, New Age International.

PAPER-III CC- 7
PHYSICAL CHEMISTRY – 2

Time : 3 Hours

Max. Marks :50 (40 for external 10 for internal)

Unit-I

Quantum Chemistry

- (a) Angular momentum** : Ordinary angular momentum, generalized angular momentum, eigenfunctions for angular momentum, eigenvalues of angular momentum, operator using ladder operations, addition of angular, momenta, spin, antisymmetry and Pauli exclusion principle.
- (b) Electronic Structure of Atoms** : Electronic configuration, Russel Saunders terms and coupling schemes, Slater- Condon parameters, term separation energies of the Pn configuration, term separation energies for the dn configurations, magnetic effects- spin orbit coupling and Zeeman splitting, introduction to the methods of self consistent field, the virial theorem.
- (c) Molecular Orbital Theory** :Huckel theory of conjugated systems, bond order and charge density calculations. Applications to ethylene. Butadiene, cyclopropenyl radical, cyclobutadiene etc.Introduction to extended Huckel theory.

Unit-II

Thermodynamics

- (a) Statistical Thermodynamics** : Concept of distribution, thermodynamics probability and most probable distribution. Ensemble averaging, postulates of ensemble and everaging. Canonical, grand canonical and micro canonical ensembles, corresponding distribution laws (using Lagrange's method of undetermined multipliers). Partition functions translational, rotational, vibrational and electronic partition functions, calculating of thermodynamic properties in terms of partition functions applications of partition functions.
- Heat capacity behaviour of solids chemical equilibria and equilibrium constant in terms of partition functions, Fermi-Dirac Statistics, Distribution law and applications to metal. Bose-Einstein Statistics- distribution law and applications to helium.
- (b) Non-Equilibrium Thermodynamics** : Thermodynamic criteria for non equilibrium states, entropy production and entropy flow, entropy balance equation 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

Macromolecules : Polymer-definition, types of polymers, electrically conducting, fire resistant, liquid crystal polymers, kinetics of polymerization, mechanism of polymerization. Molecular mass, number and

mass average, molecular mass determination (osmometry, viscometry, diffusion and light scattering methods), sedimentation, chain configuration of macromolecules, calculation of average dimensions of various chain structures.

Unit- IV Electrochemistry Part 1

Electrochemistry of solutions, Debye-Huckel-Onsager treatment and its extension, ion solvent interactions, Debye-Huckel-Jerum mode. Thermodynamics of electrified interface equations, Derivation of electrocapillarity, Lippmann equations (surface excess), methods of determination. Structure of electrified interface. Guoy-Chapman, Stern, Graham-Devanathan-Mottwatts, Tobin, Bockris, Devanathan model.

Unit-V Electrochemistry Part 2

Over potentials, exchange current density, derivation of Butler-Volmer equations, Tafel plot. Quantum aspects of charge transfer at electrodes-solution interfaces, quantization of charge transfer, tunneling.

Books 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 Kinetics, K.J. Laidler, McGraw Hill.
6. Kinetics and Mechanism of Chemical Transformations, J. Rajaraman and J. Kuriacose, McMillan.
7. Micelles, Theoretical and Applied Aspects, V. Moroi, Plenum.
8. Modern Electrochemistry Vol. 4 and Vol. II, J.O.M. Bockris and A.K.N. Reddy, Plenum.
9. Introduction to Polymer Science, V.R. Gowarikar, N.V. Vishwanathan and J. Sridhar, Wiley Easter.

Paper-IV : CC-8

ANALYTICAL CHEMISTRY -2

Time : 3 Hours

Max. Marks :50 (40 for external 10 for internal)

Unit-I

Fundamentals of Chemical Analysis:

Classification of analytical method, significance, Sensitivity and Selectivity of Analytical methods, Sampling, Accuracy & precision, Errors: types of errors, error distribution curve, avoid, standard Deviation; Calibration curve and Correlation Coefficient; linear regression; Confidence level, student 't' test, Analysis of Variance (ANOVA). Good lab practices.

Quality control, Quality assurance, International standards & government standards in chemical analysis.

Unit II

Soil and water analysis : Chemical profile of soils, definition, fertility management of soils, soil sediment analysis- physical and chemical parameters. Sources of water pollution-solid waste, industrial, agricultural, oil, radioactive waste, thermal pollution. Classification of water pollutants- basis, effects and controls. Sampling of water pollutants. Methods of analysis different parameters of soil and water analysis.

Unit-III

Electroanalytical Methods:

(a) Voltammetry of Alternating Current (AC), Linear potential sweep (DC) cyclic potential sweep voltammetry (CV) and stripping (Anodic & Cathodic) Analysis.

(b) **Thermal Analysis Methods:** Basic principles, instrumentation, experimental technique of Differential Scanning Calorimetry and Differential analysis, Thermo gravimetry, Thermo mechanical analysis, Dynamic mechanical analysis, thermometric titrimetry and direct injection Enthalpimetry.

Unit-IV

Photoelectron Spectroscopy : Basic principles; photo-electric effect, Ionization process, Koopman's theorem. Photoelectron spectra of simple molecules, ESCA, chemical information from ESCA.

Auger electron spectroscopy-basic idea.

Photoacoustic Spectroscopy : Basic principles of photoacoustic spectroscopy (PAS), PAS-gases and condensed systems, chemical and surface applications.

Theory Principle, experimental techniques and application of Microwave and NMR spectroscopy.

Unit-V

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 surfaces.

Neutron Diffraction : Scattering of neutrons by solids and liquids, Magnetic scattering, measurement techniques. Elucidation of structure of magnetically ordered unit cell.

Books Suggested:

1. Modern Spectroscopy, J.M. John Wiley.
2. Applied Electron Spectroscopy for Chemical Analysis Ed. H. Windawi and F.L Ho, Wiley Interscience.
3. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, R.V. Parish, Ellis Harwood.
4. Physical Methods in Chemistry, R.S. Drago, Saunders College.
5. Chemical Applications of Group Theory, FA. Cotton.
6. Introduction to Molecular Spectroscopy, R. Chang, McGraw Hill.
7. Basic Principles of Spectroscopy, R. Chang, McGraw Hill.

8. Theory and Applications of UV Spectroscopy, H.H. Jaffe and M. Orchin,
9. Introduction to Photoelectron Spectroscopy, P.K; Ghosh, John Wiley.
10. Introduction to Magnetic Resonance, A. Carrington and A.D. Carrington and AD. MacLachlan, Harper & Row.

Semester 2

CHEMISTRY PRACTICAL

LC-3

Lab 3

Time : 7 Hours

Max. Marks :50 (40 for external 10 for internal)

A.

Quantitative Analysis

- (a) Separation and determination of two metal ions Cu-Ni, Ni-Zn, Cu-Fe etc. involving volumetric and gravimetric methods.
- (b) Determination of DO, COD and BOD of water sample.

Chromatography:

Separation of cations and anions by

- (a) Paper chromatography
- (b) Column chromatography-ion exchange.

Detection of Added colours / preservatives etc. in commercial samples

B.

Green Synthesis / Extraction

- (a) Synthesis of Bis (acetylacetonato) Copper (II)
- (b) Synthesis of Bis (acetylacetonato) Iron (III)
- (c) Extraction from plant materials

Nanoparticles synthesis – Zn/ZnO/Ag/MnO etc.

Polarimetry:

- (i) Determination of rate constant for hydrolysis/ inversion of sugar using a polarimeter.
- (ii) Enzyme - kinetic - inversion of sucrose.

C.

Virtual Chemistry Experiments – Experiments based on AR and VR

Experiments related with molecular modeling, virtual synthesis, virtual titrations, virtual chromatography etc. can be performed.

Computational chemistry

Experiments on molecular modeling, computational chemistry, metal-drug, metal-protein interaction etc. can be performed.

Spotting

IKS : State of art in Indian Knowledge system (chemical science)

Semester 2

CHEMISTRY PRACTICAL

LC-4

Lab 4

Time : 7 Hours

Max. Marks :50 (40 for external 10 for internal)

A.

- (a) Separation, purification and identification of compounds of binary mixture (one liquid and one solid) using TLC and column chromatography.
- (b) Functional group identification – By Chemical tests, IR spectra etc.
- (c) Detection of Added colours / preservatives etc. in commercial samples
- (d) Preparation of MSDS for few commonly used chemicals.

B.

Organic Synthesis

- 1- Acetoacetic ester condensation : synthesis of ethyl-n-butylacetoacetate by A.E.E. condensation.
- 2- Cannizzaro reaction : 4-chlorobenzaldehyde as substrate.
- 3- Friedel craft's reaction : b- Benzoyl propionic acid from succinic anhydride and benzene.
- 4- Aromatic electrophilic substitutions : synthesis of p-nitroaniline and b-bromoaniline.

The products may be characterized by spectral techniques.

Quantitative Analysis:

- 1- Determination of the percentage or number of hydroxyl groups in an organic compound by acetylation method.
- 2- Estimation of amines / phenols using bromate bromide solution /or acetylation method.
- 3- Determination of Iodine and Saponification values of an oil sample.

C. Physical chemistry

Solutions

- (i) Determination of molecular weight of non- volatile and non- electrolyte by cryoscopic method and to determine the activity coefficient of an electrolyte.
- (ii) Determination of the degree of dissociation of weak electrolyte and to study of deviation from ideal behaviour that occurs with a strong electrolyte.

Conductometry :

- (i) Determination of the velocity constant, order of the reaction and energy of activation for saponification of ethyl acetate by sodium hydroxide conductometrically.

- (ii) Determination of the degree of dissociation of weak electrolyte and to study of deviation from ideal behaviour that occurs with a strong electrolyte.
- (iii) Determination of the strength of strong and weak acids in a given mixture conductometrically.
- (iv) To study the effect of solvent on the conductance of AgNO_3 / acetic acid and to determine the degree of dissociation and equilibrium constant in different solvents and in their mixtures (DMSO DMF dioxane, acetone, water) and to test the validity of Debye Huckels limiting law.

Potentiometry / pH metry:

- (i) Determination of strengths of halides in a mixture potentiometrically.
- (ii) Determination of the valence of mercurous ions potentiometrically.
- (iii) Determination of the strength of strong and weak acids in a given mixture using a potentiometer / pH meter.
- (iv) Determination of temperature dependence of EMF of a cell.
- (v) Determination of the formation constant of silver- ammonia complex and stoichiometry of the complex potentiometrically.
- (vi) Acid-base titration in a non-aqueous media using a pH meter.
- (vii) Determination of activity and activity coefficient of electrolytes.
- (viii) Determination of the dissociation constant of acetic acid in DMSO, DMF, acetone and dioxane by titrating it with KOH.
- (ix) Determination of the dissociation constant of monobasic/ dibasic acid by Albert - Serjeant method.
- (x) Determination of thermodynamic constants, ΔG , ΔS and ΔH for the reaction by e.m.f. method.

Spotting

IKS : State of art in Indian Knowledge system (chemical science)

Reference Books:

- 1- Vogel's Textbook of Quantitative Analysis, revised, J. Bassett, R.C. Denney, G.H. Jeffrey and J. Mendham, ELBS.
- 2- Experiments and Techniques in Organic Chemistry, D.P. Pasto, C Johnson and M. Miller, Prentice Hall.
- 3- Macroscale and Microscale Organic Experiments, K.L. Williamson D.C. Heath.
- 4- Systematic Qualitative Organic Analysis, H. Middleton, Edward Arnold.
- 5- Vogel's Textbook of Practical Organic Chemistry, A.R. Tatchell,
- 6- Practical Physical chemistry, A.M. James and F.E. Porichard, Longman.
- 7- Findley's Practical Physical Chemistry, B.P. Levitt, Longman.
- 8- Experimental Physical Chemistry R.C. Das and B. Behera,
- 9- Green Chemistry : An experimental study, R.K. Sharma, N. Bhojak, I.T. Sidhwani and M.K. Choudhary

M.Sc. (FINAL) CHEMISTRY
Semester 3
GENERAL PAPER CC-9:
SPECTRAL TECHNIQUES AND APPLICATIONS

Time : 3 Hours

Max. Marks :50 (40 for external 10 for internal)

Unit I

(a) Vibrational Spectroscopy : Symmetry and shapes of AB_2 , AB_3 , AB_4 , AB_5 and AB_6 , mode of bonding of ambidentate ligands, ethylenediamine and diketonato complexes, application of resonance Raman spectroscopy particularly for the study of active sites of metallo proteins.

(b) Ultraviolet and Visible spectroscopy:

Various electronic transitions (185-800nm), Beer Lambert law, effect of solvent on electronic transitions, ultraviolet bands for carbonyl compounds unsaturated carbonyl compounds dienes, conjugated polyenes. Fieser-Woodward rules for conjugated dienes and carbonyl compounds, ultraviolet spectra of aromatic and heterocyclic compounds steric effect in biphenyls.

Problems of the structure elucidation using above mentioned spectroscopic techniques.

Unit II

Infrared Spectroscopy : Instrumentation and sample handling. Characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols and amines. Detailed study of vibrational frequencies of carbonyl compounds (ketones, aldehyde, esters amides acids, anhydrides, lactones, lactams and conjugated carbonyl compounds.) effect of hydrogen bonding and solvent effect on Vibrational frequencies, overtones, combination bands and fermi resonance, FTIR, IR of gaseous, solids and polymeric materials.

Problems of the structure elucidation using above mentioned spectroscopic techniques.

Unit III

Nuclear magnetic Resonance spectroscopy : General introduction and definition, chemical shift, spin-spin interaction, shielding mechanism, mechanism of measurement, chemical shift values and correlation for protons bonded to carbon (aliphatic, olefinic, aldehydic and aromatic) and other nuclei (alcohols, phenols enols, carboxylic acids, amines, amides & mercapto). Chemical exchange effect of deuteration, complex spin-spin interaction between two, three, four and five nuclei (first order spectra,) virtual coupling stereochemistry, hindered rotation, Karplus curve variation of coupling constant with dihedral angle.

Simplification of complex. Fourier transform technique, nuclear overhauser effect (NOE) Resonance of other nuclei-F,P

Problems of the structure elucidation using above mentioned spectroscopic techniques.

Unit IV

(a) Nuclear Magnetic Resonance of Paramagnetic Substances in Solution:

The contact and pseudo contact shifts, factors affecting nuclear relaxation, some application including biochemical systems, an overview of NMR of metal nuclides with emphasis on ^{195}Pt and ^{119}Sn NMR.

Problems of the structure elucidation using above mentioned spectroscopic techniques.

(b) Carbon-13 NMR Spectroscopy : General consideration: chemical shift (aliphatic olefinic, alkyne, aromatic, hetro aromatic acid carbonyl carbon) coupling constants.

Two dimensional NMR spectroscopy - COSY, NOESY, DEPT, INEPT, APT and INADEQUATE techniques.

Problems of the structure elucidation using above mentioned spectroscopic techniques.

Unit V

Mass spectrometry : Introduction, ion production- EI, CI, FD and FAB factors affecting fragmentations, ion analysis, ion abundance. Mass spectral fragmentation of organic compounds, common functional groups, molecular ion peak, metastable peak, McLafferty rearrangement. Nitrogen rule, High resolution mass spectrometry. Examples of mass spectral fragmentation of organic compounds with respect to their structure determination.

Problems of the structure elucidation using above mentioned spectroscopic techniques.

Book Suggested :

- 1- Physical Methods for Chemistry, R.S. Drago, Saunders Company.
- 2- Structural methods in Inorganic Chemistry, E.a.v. Ebsworth, D.W.H. Rankin and S. Cradock, EIBS.
- 3- Infrared and Raman spectra : Inorganic and coordination compounds K Nakamoto Iley.
- 4- Progress in Inorganic chemistry vol., 8, ed., F.A. Cotton, Vol. 15, ed. S.J. Lippard, Wiley.
- 5- Transition Metal Chemistry ed. R.L. Carlin Vol. 3, Dekker.

- 6- Inorganic Electronic Spectroscopy, A.P.B. Lever, Elsevier
- 7- NMR, NQR, EPR and Mossbauer Spectroscopy in inorganic chemistry, R.v. Parksh, Ellis Horwood.
- 8- Practical NMR Spectroscopy, M.L. Martin Heyden.
- 9- Spectrometric identification of Organic Compounds, R.M. Silverstein, G.C. Bassler and T.C. Morrill, John Wiley.
- 10- Introduction to NMR spectroscopy, R.J. Abraham, J. Fisher and P. Loftus, Wiley.
- 11- Application of spectroscopy of Organic compounds, J.r. Dyer, Prentice Hall.
- 12- Spectroscopic Methods in Organic Chemistry, D.H. Williams, I. Fleming. Tata McGraw Hill.

Semester 3

GENERAL PAPER-CC 10

INTRODUCTION TO RECENT ADVANCES IN CHEMICAL SCIENCES

Time : 3 Hours

Max. Marks :50 (40 for external 10 for internal)

Unit I

Enzymatic Chemistry : Introduction and historical perspective, chemical and biological catalysis, remarkable properties of enzyme like catalytic power, specificity and regulation. Nomenclature and classification, extraction and purification. Fischer's lock and key and Koshland's induced fit hypothesis, concept and identification of active site by the use of inhibitors, affinity labelling and enzyme modification by site- directed mutagenesis. Enzyme kinetics, Michaelis Menten and lineweaver- burk plots, reversible and irreversible inhibition.

Mechanism of enzyme Action: Transition – State theory, orientation and steric effect, acid- base catalysis, covalent catalysis, strain or distortion. Example of some typical enzyme mechanisms for chymotrypsin, ribonuclease, lysozyme and carboxypeptidase A.

Unit II

Chemistry in nanoscience and technology

Introduction: Nanoparticles, Nanoscience and Nanotechnology: Properties of Nanomaterials; Optical & magnetic. Synthesis of nanomaterial: Chemical Approaches: Chemical reduction; sonochemical synthesis; Sol-Gel Synthesis; Self-assembly. Physical Approaches: Sputtering, Aerosol spray; Chemical vapour deposition (CVD)

Applications of Nanoscience in various fields: Pharmaceuticals, Medical & Health, Energy, Environment.

Unit III

Supramolecular chemistry:

Terminology and definitions in supramolecular chemistry. Intermolecular forces, Solvent and solution properties, solvation and hydrophobic effect. Binding constants; definition and use.

Molecular Recognition: Principle of molecular recognition, host-guest complementarity, preorganisation, chelate effect, cooperativity. Synthesis and applications of supramolecular host (crown ethers, lariat ethers, podands, cryptands, spherands, calix[n]arenes, cyclodextrine) as cation and anion binding receptors and receptors for ion-pair recognition.

Supramolecular Reactivity and Catalysis: Organocatalysis mediated through hydrogen bonding, acid-base catalysis.

Principles of molecular association and organization as exemplified in biological macromolecules like enzymes, nucleic acids membranes and model systems like micelles and vesicles. Molecular receptors and design principles, cryptands, cyclophanes calixarenes, cyclodextrines. Supramolecular reactivity and catalysis. Molecular channels and transport process. Molecular devices and nanotechnology.

Unit IV

Catalysis and Green chemistry

Introduction and basic principles, Ideal synthesis, theoretical and functional details of ecofriendly synthetic protocols with suitable examples and applications: Neat synthesis (solvent free synthesis), Non-volatile organic media and water as green media in organic transformations like ionic liquid, PEG and water, Microwave irradiation as alternative energy source for the chemical transformations, Heterogeneous catalysis/ Immobile catalysis, Ultrasound assisted synthesis.

Catalysis for Green Chemistry with examples. Catalytic oxidation using H₂O₂, Bio-catalysis, Photo-catalysis, Green reagents, Green solvents including solvent free synthesis of some organic compounds and inorganic complexes, alternative sources of energy, Green energy and sustainability.

Unit V

Medicinal chemistry

Introduction to Medicinal Chemistry. History and development of medicinal chemistry

Physicochemical properties in relation to biological action. Ionization, Solubility, Partition Coefficient, Hydrogen bonding, Protein binding, Chelation, Bioisosterism, Optical and Geometrical isomerism.

Drug metabolism

Drug metabolism principles- Phase I and Phase II.

Factors affecting drug metabolism including stereo chemical aspects

Classification, SAR, introduction and Mechanism of action of drugs for following classes:

Sulfonamides: Sulfisoxazole, Sulfapyridine, Sulfacetamide* and Sulfamethoxazole* **Antibiotics:** Penicillin: Ampicillin*, Amoxycillin. Cephalosporin: Cefazolin, Cefadroxil, Cefixime*, Tetracycline, Chloramphenicol*, Amino glycosides: Streptomycin **Antimalarials:** Chloroquine*

Antiviral: Acyclovir, Remdesivir. **Antifungal:** Clotrimazole, Miconazole, Itraconazole

Books Suggested:-

- 1- Principles of Bioinorganic Chemistry S.J. Lippard and J.M. Berg, University Science Books.
- 2- Bioinorganic chemistry, I Bertini, H.B. Gray, S.J. Lippard and J.S. Valentine, University science books.
- 3- Inorganic Biochemistry vols I and II G.L. Eichhorn Elsevier.
- 4- Progress in Inorganic Chemistry, Vols 19 and 38ed, J.J. Lippard, Wiley.
- 5- Bioorganic chemistry : A Chemical Approach to Enzyme Action, Heeermann Dugas and C. Penny, Springer-Verlag.
- 6- Understanding Enzymes, Trevor Palmer, Prentice Hall.
- 7- Enzyme Chemistry : Impact and Applications, Ed. Collin J. Sucking Chapman and Hall.
- 8- Fundamental of Enzymology, NC, Price and L. Stevens Oxford, Universtiy Press.
- 9- Immobilized Enzymes An Introduction and Application in Biotechnology, Miehael D. Trevan, John wiley.
- 10- Enzymatic Reaction Mechanisms, C. Waish, W.H. Freeman.
- 11- Enzyme Structure and Mechanism, A Fersht, W.H. Freeman.
- 12- Biochemistry : The chemical Reactions of Living Cells, D.E. Metzler, Academic Press.
- 13- Enzyme Mechnisms Ed. M.L. Page and A. Williams, Royal Society of chemistry.
- 14- Principle of Biochemistry, A.L. Lehinger, Worth Publishers.
- 15- Biochemistry . L. Stryer. W.H. Freeman.
- 16- Biochemistry, J. David Rawn, Neil Patterson.
- 17- Biochemistry, Voet and Voet, John wiley.
- 18- Outline of Biochemistry, E.E. Conn and P.K. Stumpt, John Wiley.
- 19- Bioorganic Chemistry : A Chemical Approach to Enzyme Action. H. Dugas and C. Penny, Springer-Verlag.
- 20- Macromolecules : Structure and Function, F. Woold, Prentice Hall.

M.Sc. (FINAL) CHEMISTRY

Semester 3

ELECTIVE PAPERS

Group-A

PAPER : CC-11-A

ADVANCED INORGANIC CHEMISTRY Part 1

Time : 3 Hours

Max. Marks :50 (40 for external 10 for internal)

Unit-I

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

(b) Transition Metal Compounds with Bonds of Hydrogen.

Unit-II

Transition Metal π - Complexes : Transition Metal π -complexes with unsaturated organic molecules, alkenes, alkynes, allyl, diene, dienyl, arene and trienyl complexes preparations, properties, nature of bonding and structural features, important reactions relating to nucleophilic and electrophilic attack on ligands and to organic synthesis.

Unit-III

Homogenous Catalysis: Stoichiometric reactions for catalysis, homogeneous catalytic hydrogenation, Zeigler- Natta polymerization of olefins, catalytic reactions involving carbon monoxide such as hydrocarbonylation of olefins (oxo reactions), oxopalladation reactions, activation of C-H bond.

Unit-IV

Metalloenzymes: Zn enzymes-Carboxypeptidase and carbonic anhydrase. Iron enzyme catalase, peroxidase and cytochrome P-450

Copper enzyme –superoxide dismutase. Molybdenum oxatransferase enzyme aniline oxidase. Coenzyme vitamin B12 .

Unit-V

Supramolecular Chemistry : Concepts and language.

Molecular recognition : Molecular receptors for different types of molecules including anionic substrates, design and synthesis of coreceptor molecules and multiple recognition.

Books Suggested :

- 1- Principles and application of Organotransition Metal chemistry, J.P. Collman, L.S Hedder, J.R. Norton and R.G. Finke, University Science books.

- 2- The Organometallic chemistry of the Transition Metals, R.H. Crabtree John Wiley.
- 3- Metallo- Organic Chemistry, A.J. Pearson, Wiley.
- 4- Organometallic Chemistry, R.C. Mehrotra and A. Singh, New Age International.
- 5- Principles of Bioinorganic Chemistry, S.J. Lippard and J.M. Berg, University Science Books.
- 6- Bioinorganic Biochemistry, I. Bertini, H.B. Gray, S.J. Valentine, University Science Books.
- 7- Inorganic Biochemistry vols I and II G.L. Eichhorn Elsevier.
- 8- Progress in Inorganic Chemistry, Vols 18 and 38 ed. J.J. Lippard, Wiley.
- 9- Supramolecular Chemistry, J.M. Lehn, VCH

Semester 3

ELECTIVE PAPERS

Group-A

PAPER : CC-12-A

METAL COMPLEXES AND POLYMERS

Time : 3 Hours

Max. Marks :50 (40 for external 10 for internal)

Unit-I

Basics of Photochemistry : Absorption, excitation, photochemical laws, quantum yield, electronically excited states life times-measurements of the times. Flash photolysis. Stopped flow technique Energy dissipation by radiative and non-radiative processes. Absorption spectra, Frank-Condon principle, photochemical stages- primary and secondary process.

Unit-II

Properties of Excited States : Structure, dipole moment, acid-base strengths, reactivity. Photochemical kinetics, calculation of rates of radiative processes. Bimolecular deactivation- quenching.

Excited states of Metal Complexes: Excited states of metal complexes, Comparison with organic compounds, electronically excited states of metal complexes, charge – transfer spectra, charge transfer excitations, methods for obtaining charge – Transfer spectra.

Unit-III

Redox Reaction by Excited Metal complexes : Energy transfer under condition of weak interaction and strong interaction- exciplex formation; conditions of the excited states to be useful as redox reactants, excited electron transfer, metal complexes as attractive candidates (2, 2' bipyridine and 1, 10 phenanthroline complexes), illustration of reducing and oxidizing character of Ruthenium 2 (bipyridyl complex, comparison with Fe (bipy)₃ role of spin orbit coupling life time of these complexes. Application of redox processes of electronically excited states for catalytic purpose, transformation of low energy reactants into high energy products, chemical energy into light.

Unit IV

Metal complex sensitizers : Metal complex sensitizer, electron relay, metal colloid system, semiconductor supported metal or oxide system, water photolysis, nitrogen fixation and carbon dioxide reduction.

Unit-V

Polymer characterization : polydispersion – average molecular weight concept. Number, weight and viscosity average molecular weights Polydispersity and molecular weight distribution. The practical significance of molecular weight measurement of molecular weights. End-group, viscosity light scattering, osmotic and ultracentrifugation methods, X-ray diffraction study Microscopy. Thermal analysis and physical testing – tensile strength. Fatigue, impact. Tear resistance. Hardness and abrasion resistance.

Books Suggested :

- 1- Concepts of inorganic photochemistry, A.W. Adamson and P.D. Fieschauder, Wiley.
- 2- Inorganic Photochemistry, J. Chem. Educ. Vol. 60, No10, 1983
- 3- Progress in inorganic chemistry, vol 30 ed, S.J. Lippard Wiley.
- 4- Coordination Chem. Revs. 1981, vol39, 121, 131, 1975, 15, 321, 1970 97, 113
- 5- Photochemistry of Coordination Compounds, V. Balzani and V. Carassiti Academic press.
- 6- Elements of inorganic photochemistry, G.J. Willey.
- 7- Textbook of polymer Science, FW Lamba, Prentice Hall
- 8- Physical and Chemistry of polymers, J.M.G. Cowie, Blackies Academic and Professional.
- 9- Functional monomers and polymers, K. Takemoto, Y. Inaki and RM Ottanbrite.
- 10- Contemporary polymers Chemistry, H.R. Alcock and F.W. Lambe, Prentice Hall.
- 11- Polymers of science V.R. Gowarikar, N.V. Vuswanathan and J. Sreedhar Wiley- Eastern.

Semester 3

ELECTIVE PAPERS

Group-B

PAPER : CC-11-B

ORGANIC SYNTHESIS Part 1

Time : 3 Hours

Max. Marks :50 (40 for external 10 for internal)

Unit-I

Organometallic Regents : Principles, preparations, properties and applications of the following in organic synthesis with mechanistic details.

Group I and II Metal organic compounds : Li, Mg, Hg, Cd, Zn, and Ce compounds

Unit-II

Advanced applications of Organometallic Regents of Transition Metals : Cu, Pd, Ni, Fe, Co, Rh, Cr, and Ti compounds

Unit-III

Oxidation : Introduction, different oxidative processes. Hydrocarbons – Alkenes aromatic rings, saturated C-H groups (activated and unactivated)

Alcohols, diols, aldehydes, ketones and carboxylic acids Amines, hydrazines and sulphides. Oxidations with Ruthenium tetroxide, Iodobenzene diacetate and Thallium (III) nitrate.

Unit-IV

Reduction : Introduction, different reduction processes. Hydrocarbons- Alkanes, alkenes, alkynes and aromatic rings. Carbonyls compounds- aldehydes, ketones, acids and their derivatives, Epoxides. Nitro, Nitroso, Azo and oxime groups. Hydrogenolysis.

Unit-V

Rearrangements : General mechanistic considerations – nature of migration, migratory aptitude. Memory, effects. A detailed study of the following rearrangements- Pinacol- pinacolone, Wagner-Meerwein, Diels-Alder, Benzil- Benzilic acid, Favorskii, Arndt- Eistert synthesis, Neber, Beckmann, Hofmann, Curtius Schmidt, Baeyer- Villiger, Shapiro reaction. Metallocenes, non Benzenoid aromatics and Polycyclic Aromatics compounds general considerations, synthesis and reactions of some representative compounds.

Books Suggested :

- 1- Modern Synthetic Reactions, H.Q. House, W.A. Benjamin.
- 2- Some modern Methods in organic synthesis, W. Carruthers, Cambridge University Press.
- 3- Advanced Organic Chemistry reactions mechanisms and structure J March John Wiley.
- 4- Principles of Organic Synthesis, R.C. Norman and J.M. Coxon, Blackie Academic & Professional.
- 5- Advanced organic chemistry Part-B, F.A. Carey and R.J. Sundberg Plenum Press.
- 6- Rodd's chemistry carbon compounds, ed S. Coffey, Elsevier.
- 7- Designing organic synthesis S Warren Wiley.
- 8- Organic synthesis – concepts, methods and starting materials J Furrow and G. Penzillan, VCH.
- 9- Some modern methods of organic synthesis W.E. Carruthers Cambridge University Press.
- 10- Modern synthesis reactions, H.Q. House W.A.A. Benjamin.
- 11- Advanced organic chemistry reactions, Mechanisms and structure, March Wiley
- 12- Principles of organic synthesis, R.C. Norman and J.M. Cozon, Blackie Academic & Professional.
- 13- Advanced organic chemistry Part-B.F.A Carey and R.J. Sundberg. Plenum Press.

Semester 3

ELECTIVE PAPERS

Group-B

PAPER : CC-12-B

HETEROCYCLICS AND NATURAL PRODUCTS Part 1

Time : 3 Hours

Max. Marks :50 (40 for external 10 for internal)

Unit-I

(a) Nomenclature of Heterocycles : Systematic nomenclature (Hantzsch – Widman system) for monocyclic, fused and bridged heterocyclics.

(b) Aromatic Heterocycles : General chemical behaviour of aromatic heterocycles , classifications (Structural type), criteria of aromaticity (bond lengths, ring current and chemical shifts in H NMR- spectra, empirical resonance energy, delocalization energy and Dewar resonance energy, diamagnetic susceptibility exaltations).

Unit II

Non aromatic Heterocycles : strain in bond angle and torsional strain and their consequences in small ring heterocycles.

Conformation of six-membered heterocycles with reference to molecular geometry, barrier to ring inversion, pyramidal inversion and 1,3- diaxial interaction.

Stereo- electronic effects, anomeric and related effects. Attractive interaction hydrogen bonding and intermolecular nucleophilic electrophilic interactions.

Unit III

Heterocyclic Synthesis : Principles of heterocyclic synthesis involving cyclization reaction and cycloaddition reactions with reference to synthesis and reactions of aziridines, oxiranes, thiranes, azetidines, oxetanes and thietanes.

Unit IV

Benzo- Fused Five Membered Heterocycles : Synthesis and reactions including medicinal applications of benzopyrroles, benzofuranes and benzothiophenes.

Unit V

Seven- and large membered Heterocycles : synthesis and reactions of diazepines, thiazepines, azocines, diazocines, dioxocines and dithiocine.

Books Suggested :

- 1- Heterocyclic chemistry Vol, 1-3, R.R. Gupta, M. Kumar and V. Gupta springer Verlag.
- 2- The Chemistry of Heterocycles, T. Eicher and S. Hauptmann, thieme.
- 3- Heterocyclic chemistry, J.A. Joule, K. Mills and G.F. Smith, Chapman and Hall.
- 4- Heterocyclic Chemistry, T.L. Gilchrist, Longman Scientific Technical.
- 5- Contemporary Heterocyclic compounds, R.M. Acheson, John Wiley.

- 6- An introduction to the Heterocyclic compounds R.M. Acheson, John Wiley.
- 7- Comprehensive Heterocyclic Chemistry, A.R. Katritzky and C.W. Reeds, ed. Pergamon Press.
- 8- Natural Products : chemistry and Biological Significance, J Mann, R.S. Davidson, J.B. Hobbs, D.V. Banthorpe and J.B. Harborn, Longman Essex.
- 9- Organic Chemistry, Vol2, I.L. Finar Elbs.
- 10- Stereoselective synthesis : A practical Approach, M. Nogradi, BCH.
- 11- Rodd's Chemistry of Carbon Compounds, Ed. S. Coffey, Elsevier.
- 12- Chemistry, biological and Pharmacological Properties of Medicinal Plants from the Americas, Ed Kurt Hostettmann, M.P Gupta and A. Marston, Harwood Academic Publishers.
- 13- Introduction to Flavonoids, B.A. Bohm, Harwood, Academic Publishers.
- 14- New trends in natural products chemistry Atta- Ur Rahman and M.L. Choudhary, Harwood Academic Publishers.
- 15- Insecticides of Natural Origin Sukhdev, Harwood Academic Publishers.

Semester 3

ELECTIVE PAPERS

Group-C

PAPER : CC-11-C

**RECENT TRENDS IN PHYSICAL CHEMISTRY Part 1
(PHYSICAL-ORGANIC CHEMISTRY)**

Time : 3 Hours

Max. Marks :50 (40 for external 10 for internal)

Unit I

Principle of Reactivity: Mechanistic significance of entropy, enthalpy and Gibbs free energy, Arrhenius equation. Transition state theory, uses of activation parameters, Hammond's postulate, Bell Evans- Polanyi principles. Potential energy surface model, Marcus theory of electron transfer reactivity and selectivity principles.

Unit II

Radical and Pericyclic Reactivity : Radical stability, polar influences, solvent and steric effect. A curved approach to radical addition, factors affecting barrier heights in additions, regioselectivity in radical reactions. Reactivity, specificity and periselectivity in pericyclic reactions.

Unit III

Acids, Bases, Electrophiles, Nucleophiles and Catalysis: Acid base dissociation. Electronic and structural effects, acidity and basicity. Acidity functions and their applications. Hard and soft acids and bases. Nucleophilicity scales. Nucleofugacity. The α effect. Ambivalent nucleophiles. Acids base

catalysis specific and general catalysis. Bronsted catalysis. Nucleophilic and electrophilic catalysis. Catalysis by non covalent binding- micellar catalysis.

Unit IV

Solvation and solvent Effects : Qualitative understanding of solvent solute effects on reactivity. Thermodynamic measure of solvation. Effects of solvation on reaction rates and equilibria. Various empirical index of solvation based on physical properties, solvent- sensitive reaction rates, spectroscopic properties and scale for specific solvation. Use of solvation scales in mechanistic studies, Solvent effects from the curve crossing model.

Kinetic Isotope Effect : Theory of isotope effects, primary and secondary kinetic isotope effects. Heavy atom isotope effects. Tunnelling effect, solvent effects.

Unit V

Structural effects on reactivity : Linear free energy relationships (LFER). The Hammett equation, substituent constant, theories of substituent effects. Interpretation of ρ Values, reaction constant ρ . Deviation from Hammett equation, Dual parameter correlations, inductive substituent constant. The Taft model, σ_1 and σ_R scale.

Steric and Conformational properties : Various type of steric strain and their influence on reactivity. Steric acceleration. Molecular measurements of steric effects upon rates. Steric LFER. Conformational barrier to bond rotation spectroscopic detection of individual conformers. Acyclic and monocyclic systems.

Rotation around partial double bonds. Winstein-Holness and Curtin-Hammett Principle.

Book Suggested :

- 1- Molecular Mechanics, U Burkert and N.L. Allinger, ACS Monograph 177, 1982.
- 2- Organic Chemists' book of orbitals. L Salem and W.L. Jorgensen, Academic Press.
- 3- Mechanism and Theory in Organic Chemistry, T.H. Lowry and K.C. Richardson, Harper and Row.
- 4- Introduction to Theoretical Organic Chemistry and Molecular. Modeling, W.B. Smith, VCH Weinheim.
- 5- Physical Organic Chemistry, N.S. Lissacs, ELBS/Longman.
- 6- Supramolecular Chemistry, Concepts and Perspective, J.M. Lehn, VCH.
- 7- The physical Basis of Organic Chemistry, H. Haskill, Oxford University Press.
- 8- An introduction to Liquid State, P.A. Egelstaff, Academic Press.
- 9- The Dynamic State, A.F.M. Barton, Longman.
- 10- Introduction to Statistical Thermodynamics T.L. Hill Addison Wiley.
- 11- The Liquid State, J.A. Pryde.
- 12- Significant Liquid Structures, H. Eyring and M.S. John

Semester 3

ELECTIVE PAPERS

Group-C

PAPER : CC-12-C

ADVANCES IN ELECTROCHEMISTRY

Time : 3 Hours

Max. Marks :50 (40 for external 10 for internal)

Unit-I

Semiconductor interfaces: Theory of double layer at semiconductor-electrolyte solution interfaces, structure of double layer interfaces, limiting current in semiconductor electrodes, effect of light at semiconductor solution interface.

Unit-II

Electro catalysis and Bioelectrochemistry

chemical catalyst and electrochemical catalysts, Electrocatalysis in simple redox reactions, in reaction involving adsorbed species. influence of various parameters. Bioelectrode, threshold membrane phenomena, Nernst-Planck equation, Hodge-Huxley equations, core conductor models, electrocardiography. Enzymes as electrodes

Unit-III

Introduction to corrosion, homogeneous theory, forms of corrosion. Thermodynamics and the stability of metals, potential- pH (or Pourbaix) diagram: uses and abuses. Corrosion current and corrosion potential – Evans diagrams.

Unit-IV

Measurement of corrosion rate: (i) weight loss method (ii) electrochemical method. cathodic corrosion monitoring and prevention methods and anodic protections (i) inhibition by addition of substances to the electrolyte environment (ii) by charging method from external source, anodic protection, organic inhibitors. The fuller story green inhibitors

Unit-V

Conversion And Storage of Electrochemical Energy: electrochemical energy converters, maximum intrinsic efficiency of an electrochemical converter physical interpretation of the Carnot efficiency factor in electrochemical energy converters. Power outputs.

storage cells, fuel cells, solar cells Types of storage cells (batteries) ,measure of cell performance, Properties of electrochemical energy storers: measure of battery performance, charging and discharging of battery, , introduction of classical batteries , modern batteries –zinc-air , nickel-metal oxide and lithium batteries. Brief history of fuel cells, efficiency of fuel cells, hydrogen-oxygen fuel cell, phosphoric acid fuel cell, direct methanol and biochemical fuel cells; Solar cells introduction, principle and working of solar cells, advantages.

Book Suggested :

- 1- Computational Chemistry, A.C. Norris, John Wiley.
- 2- Computer Programming in FORTRAN 77, R Rajasthan, Prentice Hall.
- 3- Numerical Analysis, CE. Frogberg, Macmillan.
- 4- Numerical Analysis-A Practical Approach, M.J. Meron, John Wiley.
- 5- Numerical Methods for scientists and Engineers H.M. Antia Tat Mcgrow Hill.
- 6- Modern Quantum Chemistry N.S. Ostlund and A. Szabo, McGraw Hill.
- 7- Methods of Molecular Quantum Mechanics, R. Mcweeny and B.T. Sutcliffe, academic Press.
- 8- Density Functional Theory of Atoms and Molecules, RG. Parrand W Yang, Oxford.
- 9- Exploring Chemistry with Electron Structure Methods, JB. Foresman and E. Frish Goussian Inc.
- 10- Semi-Empirical MO Theory, J. Pople and D.L. Beveriadge.

Semester 3

ELECTIVE PAPERS

Group-D

PAPER : CC-11-D

ANALYTICAL CHEMISTRY Part 1

Time : 3 Hours

Max. Marks :50 (40 for external 10 for internal)

UNIT-I

Instrumental Methods- Classification of techniques, important consideration, measurement of data sensitivity and detection limit, Noise, Signal to noise ratio, Accuracy and instrument calibration, Evaluation results by statistical methods.

Unit II

Computer Aided Analysis: Computer organization -Software & Hardware, interfacing computers in instruments.

Process control & Laboratory Analyzer: Industrial process analyzers- Infrared, Oxygen, potentiometric and gas-chromatographic, online process control, Automatic chemical analyzer and element (C,H,N,O) analyzer.

UNIT-III

Spectral methods of Analysis-

- (a) Raman Spectroscopy- Theory, Instrumentation, experimental technique and structural analysis.
- (b) Infrared Spectroscopy, Sample handling, Instrumentation, experimental technique, qualitative and quantitative analysis, FT-IR & NIR.
- (c) Mass-Spectrometry:- Mass,spectrometry, Sample flow, inlet sample system, ionization methods, mass analyzers, ion-collection system , experimental technique andcorrelation of Mass spectra with molecular structure.

UNIT-IV

X-Ray Spectra:- Instrumentation, experimental technique of X-Ray analysis–Direct, X-ray Diffraction (XRD), Absorption(XRA) & Fluorescence (XRF)

UNIT-V

Electron Microscopy: Types (TEM,SEM,REM and LVEM), sample preparation and application in life sciences ,industries and research Scanning and Transmission Electron Microscopy

Books Suggested :

- 1- Analytical Chemistry, G.D. Christian, J. Wiley.
- 2- Fundamentals of Analytical Chemistry, D.A. Skoog,, D.M. Westand F.J. Holler, W.B. Saunders.
- 3- Analytical Chemistry – Principles, J.H. Kennedy, W.B. Saunders.
- 4- Analytical chemistry – Principles and techniques, LG. Hargis, Prentice Hall.
- 5- Principles of Instrumental Analysis, D.A. Skoog, J.L. Loary, W.B. Saunders.
- 6- Principles of Instrumental Analysis, D.A. Skoog, W.B. Saunders.
- 7- Quantitative Analysis, R.A. Day, Jr. and A.L. Underwood Prentice Hall.
- 8- Basic Concepts of Analytical Chemistry, S.M. Kholkar, Wiley Eatern.
- 9- Handbook of Instrumental Techniques for Analytical Chemistry, F. Settle Prentice Hall.

Semester 3

ELECTIVE PAPERS

Group-D

PAPER : CC-12-D

APPLIED ANALYTICAL CHEMISTRY Part 1

Time : 3 Hours

Max. Marks :50 (40 for external 10 for internal)

Unit-I

Pharmaceutical Analysis:- Introduction to drugs, their classification, sources of impurities in pharmaceutical raw materials such as chemical, atmospheric and microbial contaminants etc. Limit tests for impurities like, Pb, As, Fe, moisture, chlorides, sulfates, Boron, free halogen, selenium etc. Analysis of some commonly used drugs like sulfadugs, antihistamines, barbiturates, vitamins (A, B6, C , E, K) etc.

Unit-II

Clinical Analysis : Composition of blood, collection, and preparation of samples, clinical analysis – serum electrolytes, blood glucose, blood urea nitrogen , uric acid , albumin , globulin , barbiturates , acidic and alkaline phosphates , Immunoassay , principals of radio immunoassay, and applications . The blood gas analysis – trace elements in the body. Drug analysis: Narcotics and dangerous drugs, classification of drugs, screening by gas and thin layer chromatography and spectrophotometric analysis

Unit-III

Analysis of soil and fertilizers: Moisture, pH, total nitrogen, phosphorous, silica, lime, Magnesia, Manganese, sulfur & alkali salts. Method of soil analysis, soil fertility its determination, determination of inorganic constituents of plant materials, Chemical analysis as measure of soil fertility, analysis of fertilizers.

Unit-IV

Fuel Analysis:- Solid, liquid and Gas Fuels:- Solid Fuels: ultimate and proximate analysis, heating values, grading of coal. Liquid fuels: flash points, aniline point, octane number and carbon residue, Gaseous fuels: producer gas and water gas – calorific value.

Unit-V

Food analysis: Moisture, ash, crude protein, fat, crude fiber, carbohydrate, calcium, potassium, sodium, and phosphates, food adulteration – common adulteration in food, contamination of food stuffs, microscopic examination of foods for adulterants, Pesticide analysis in food products, Extraction and purification of sample, HPLC, gas chromatography for organo – phosphates, thin layer chromatography for identification of chlorinated pesticides in food products.

Reference Books:

1. F. J. Welcher: Standard methods of Chemical analysis, 6th Ed. Vol. I and II (D. Van Nostrand Comp.)
2. I. M. Kolthoff: Treatise on Analytical Chemistry Vol. I & II
3. F. D. Snell: Encyclopedia of industrial Chemical Analysis Vol. 1 to 20 (John Wiley)
4. Riech: Outline of Industrial Chemistry.
5. K. H. Buchel: Chemistry of Pesticides (John Wiley)
6. Nichollas: Aids to the Analysis of foods and Drugs.
7. A. H. Beckett and J. B. Stanlake; Practical Pharmaceutical Chemistry Vol. I & II (CBS publishers)
8. S. Ranganna: Handbook of analysis and quality control for fruits and vegetable products (McGraw Hill)
9. Ramalu: Analysis of pesticides
10. Bassett, Denney-Jeffer and Mendham, Vogel's Textbook of Quantitative Inorganic Analysis, (5th edition).
11. A.K. De : Standard Methods of Waste and Waste water analysis.
12. S.M. Khopkar, Environmental Chemistry ; Environmental pollution analysis.
13. M.S. Creos and Morr, Environmental Chemical Analysis, American publication (1988)
14. A.K. De, Environmental Chemistry, New Age International publishers. Moghe and
15. Ramteke, Water and waste water analysis : (NEERI)
16. A.C. Stern, Air pollution: Engineering control vol. IV (AP)
17. P.N. Cheremisinoff and R.A. Young, Air Pollution control and Design. Hand Book Vol. I & II (Dekker)
18. B.K. Sharma, Industrial Chemistry.
19. S.P. Mahajan, Pollution Control in Process Industries.
20. R.A. Horne, Chemistry of our Environment.
21. Ruzica and Stary, Substoichiometry in Radiochemical Analysis. Pergamon.

22. Ladd and Lee, Radiochemistry.
23. Clerk, Handbook of Radiochemical methods
24. Hillebrand Lhundel, Bright and Hoffman, Applied Inorganic Analysis, John Wiley.
25. Snell and Biffen, Commercial Methods of Analysis.
26. P.G. Jeffery, Chemical Methods of Rock Analysis, Pergamon.
27. Allan Cury, Irvins Sunshine, Forensic Analysis, Academic Press Publications.
28. Karamer Twig: Quality control for food industry (AVI)
29. G. F. Longonan: the analysis of detergents and detergent products (JW)
30. A. Davidsohn & B. M. Mlwidaky : Synthetic detergents (Book center, Mumbai)
31. Chopra and Kanwar, Analytical Agriculture Chemistry, Kalyani Publishers.
32. Aubert and Pintes, Trace Elements in Soils.
33. Bear, Chemistry of Soil.
34. Hauson, Plant Growth Regulators, Noyes.

Semester 3

ELECTIVE PAPERS

Group-A

PRACTICAL PAPER : LC-5-A

CHEMISTRY LAB 5A

Time : 7 Hours

Max. Marks :50 (40 for external 10 for internal)

INORGANIC CHEMISTRY

A. Preparations

(Minimum seven – identification and characterization should be on the basis spectral techniques)

1. Sodium amide
2. Metal Oxalates.
3. Alums.
4. Trialkoxyboranes.
5. PhBCl_2 dichlorophenylborane-Synthesis in vacuum line.
6. Tin Iodides / Tin complexes
7. Lead complexes
8. Hexa-bis (4-Nitrophenox cyclotriphosphazene.)
9. Synthesis of trichlorodiophenylantimony (V) hydrate
10. Sodium tetrathionate $\text{Na}_2\text{SO}_4\text{O}_8$.
11. Metal complexes of Ir / Ru / Rh
12. Synthesis of metal acetylacetonate,
13. Bromination of $\text{Cr}(\text{acac})_2$.

14. Magnetic moment of $\text{Cu}(\text{acac})_2 \cdot 2\text{H}_2\text{O}$.
15. Separation of optical isomer of $\text{cis-}[\text{Co}(\text{en})_2\text{Cl}_2]\text{Cl}$.

B. Chromatographic Separations (Any Three)

TLC / PC / HPTLC/ CC/ GC / HPLC – at least three should be used

- a. Cadmium and Zinc.
- b. Zinc and Magnesium
- c. Nickel and Manganese
- d. Cobalt and zinc.
- e. Complex mixture can be used

C. Green methods (at least one from extraction, synthesis and analysis)

Spotting

In spotting there should be 5 spots related with instruments and techniques as per syllabus ; time of spotting is 20 minutes

IKS : Applied Chemical Science / Technology in Indian Knowledge system

Semester 3

ELECTIVE PAPERS

Group-A

PRACTICAL PAPER : LC-6-A

CHEMISTRY LAB 6A

Time : 7 Hours

Max. Marks :50 (40 for external 10 for internal)

INORGANIC CHEMISTRY

A. Preparation (Minimum seven)

1. Ion exchange separation of oxidation state of vanadium.
2. Determination of Cr (III) complexes $[\text{Cr}(\text{H}_2\text{O})_6] \text{NO}_3 \cdot 3\text{H}_2\text{O}$, $[\text{Cr}(\text{H}_2\text{O})_4 \text{Cl}_2] \text{Cl} \cdot 2\text{H}_2\text{O}$, $[\text{Cr}(\text{en})_3] \text{Cl}_3$, $\text{Cr}(\text{acac})_3$
3. Preparation of N. N bis (salicylaldehyde) ethylenediamine, salen H_2 , $\text{Co}(\text{Salen})$
4. Preparation of Fe (II), chloride (use it as Friedal- Craft chlorination)
5. Reaction of Cr. (III) with a multidentate ligand a kinetics experiments
6. Preparation of $[\text{Co}(\text{phenanthroline-5,6-quinone})]$.
7. Preparation and use of Ferrocene.
8. Preparation of copper glycine complex-cis and trans bis glycinato cooper (II).
9. Preparation of Phosphine Ph_3P and its transition metal complexes.

10. Conversion of p-xylene to terephthalic acid catalyzed by CoBr_2 (homogeneous catalysis).
11. Preparation of any other Inorganic Compound of more difficult type.
12. Green Synthesis of fluorescent isomers of tris (8-hydroxyquinolato) aluminium (III)
13. Green Synthesis of Synthesis of Bis (acetylacetonato) Manganese (III)
14. Green Synthesis of any organometallic compound

B. Analytical Techniques (at least five)

Prepared and selected inorganic compounds should be analyzed and studied by IR, electronic spectra, Mossbauer, ESR, magnetic susceptibility measurements.

Handling of air and moisture sensitive compounds involving vacuum lines should be demonstrated.

C. Primary information / experimentations on Indian pharmacopoeia, Ayurvedic pharmacopoeia, BIS methods and ISO methods

Project & Seminar

The project work should be allotted by a committee constituted at the institute level in the beginning of the semester III. The project should be based on syllabus / local problem / industry / institution. The project should have interdisciplinary approach. The presentation should be in front of a panel and a proper record with geotagged photographs should be maintained.

Semester 3

ELECTIVE PAPERS

Group-B

PRACTICAL PAPER : LC-5-B

CHEMISTRY LAB 5B

Time : 7 Hours

Max. Marks :50 (40 for external 10 for internal)

A. Organic Analysis and Synthesis

(a) **Qualitative Analysis** :- Separation, purification and identification of the components of mixture of three organic compounds (three solids or two liquids and one solid, two solids and one liquid) using TLC for checking the purity of the separated compounds. Chemical analysis.

(b) Multi-Step Synthesis of Organic Compounds

- a. Photochemical reactions : Benzophenone benzpinacol benzpinacolone
- b. Beckmann rearrangement :
- c. Benzilic acid rearrangement Benzilic acid from benzoin.
- d. Synthesis of heterocyclic compounds Skraup synthesis : preparation of quinoline from aniline
Fisher-Indole synthesis : preparation of 2-phenylindole from phenylhydrazine.

NOTE —Other similar synthesis of three steps.

B. Green methods (at least one from extraction, synthesis and analysis)

C. Analytical Techniques (at least five)

Prepared and selected organic compounds should be analyzed and studied by –

IR, Uv-vis, NMR, Mass, GC-Mass, HPLC, HPTLC, TLC, CC.

Handling of air and moisture sensitive compounds involving vacuum lines should be demonstrated.

Spotting

In spotting there should be 5 spots related with instruments and techniques as per syllabus ; time of spotting is 20 minutes

IKS : Applied Chemical Science / Technology in Indian Knowledge system

Semester 3

ELECTIVE PAPERS

Group-B

PRACTICAL PAPER : LC-6-B

CHEMISTRY LAB 6B

Time : 7 Hours

Max. Marks :50 (40 for external 10 for internal)

A. Multi-Step Synthesis of Organic Compounds (Any Four)

The exercise should illustrate the use of organic reagents and may involve purification of the products by chromatography techniques.

- Enzymatic synthesis- enzymatic reduction ; Reduction of ethyl acetoacetate using Baker's yeast to yield enantiomeric excess of S(+) ethyl-3-hydroxybutanoate and determine its optical purity.
- Biosynthesis of ethanol from sucrose.
- Synthesis using microwaves Alkylation of diethyl malonate with benzyl chloride.
- Synthesis using phase transfer catalyst.
- Alkylation of diethyl malonate or ethyl acetoacetate with an alkyl halide.
- Green synthesis / Solvent free Aldol condensation and
- Benzoin condensation with thiamine as a catalysts instead of cyanide

NOTE —Other similar synthesis of three steps.

B. Extraction of Organic Compounds from Natural Sources (Any Five)

- Isolation of caffeine from tea leaves.
- Isolation of casein from milk (the students are required to try some typical colour reactions of proteins).
- Isolation of lactose from milk (purity of sugar should be checked by TLC and PC and R_f value reported).
- Isolation of nicotine dipicrate from tobacco.

5. Isolation of cinchonine from cinchona bark.
6. Isolation of piperine from black pepper.
7. Isolation of lycopene from tomatoes.
8. Isolation of β -carotene from carrots.
9. Isolation of oleic acid from olive oil (involving the preparation of complex with urea and separation of linoleic acid).
10. Isolation of eugenol from cloves.
11. Isolation of (+) limonene from citrus rinds.

C. Primary information / experimentations on Indian pharmacopoeia, Ayurvedic pharmacopoeia, BIS methods and ISO methods.

Project & Seminar

The project work should be allotted by a committee constituted at the institute level in the beginning of the semester III. The project should be based on syllabus / local problem / industry / institution. The project should have interdisciplinary approach. The presentation should be in front of a panel and a proper record with geotagged photographs should be maintained.

Semester 3

ELECTIVE PAPERS

Group-C

PRACTICAL PAPER : LC-5-C

CHEMISTRY LAB 5C

Time : 7 Hours

Max. Marks :50 (40 for external 10 for internal)

A. Experiments based on Conductivity measurements:

1. Conductometric Titration: Acid-base, Precipitation and complex salts.
2. To determine the equivalent conductance of a weak electrolyte at different concentrations and hence test the validity of Ostwald's dilutions law. Also determine the dissociation constant of the weak electrolyte.
3. To determine the equivalent conductance of a strong electrolyte at several dilutions, and hence verify the Onsager equation.
4. To determine the equivalent conductance of a weak electrolyte at infinite dilution using the Kohlrausch law.
5. To determine the solubility of a sparingly soluble salt in water by conductance measurement.

6. To determine the basicity of an organic acid by conductometric measurement.
7. To determine the composition of a mixture of acetic acid and hydro chloric acid by conductometric titration.
8. To determine the degree of hydrolysis and hydrolysis constant of salts (e.g. CH_3COONa , NH_4Cl)
9. Determination of hydrolysis constant of aniline hydrochloride.
10. Titration of a solution of a salt of a weak base and strong acid, say NH_4Cl

B Experiments based on Potentionmetric and pH measurements:

1. Potentiometric and pH metric titrations: Acid-base, oxidation-reduction and complex salts.
2. Titration of a mixture of HCl and CH_3COOH and hence the composition of the mixture.
3. Titration of a mixture of CH_3COOH and CH_3CoNa and to determine the dissociation constant of the acid.
4. To determine the ionization constants of a polybasic acid (H_3PO_4).
5. To determine the solubility and solubility Product of AgCl , AgBr and AgI .
6. To determine the hydrolysis constant of aniline hydrochloride.
7. Determine the composition of a given mixture containing KCl and KI .
8. Determination of acid, and basic dissociation constants of an amino acid, and hence the iso-electric point of the acid.
9. To determine the solubility product of silver halide (AgCl)
10. Determination of Ionic product of water.

C. Primary information / experimentations on Indian pharmacopoeia, Ayurvedic pharmacopoeia, BIS methods and ISO methods

Spotting

In spotting there should be 5 spots related with instruments and techniques as per syllabus ; time of spotting is 20 minutes.

IKS : Applied Chemical Science / Technology in Indian Knowledge system

Semester 3

ELECTIVE PAPERS

Group-C

PRACTICAL PAPER : LC-6-C

CHEMISTRY LAB 6C

Time : 7 Hours

Max. Marks :50 (40 for external 10 for internal)

A Experiments based on Kinetics:

1. To study the nature of salt effect on $\text{S}_2\text{O}_8^{2-}$ -I reaction and conclude the nature of the species in the slow step.
2. To investigate the inversion of cane sugar in presence of an acid. Determine the energy of activation of the reaction.
3. To study the kinetics of hydrolysis of ethyl acetate by NaOH at two temperatures by conductance measurement, and hence the energy of activation of the reaction.
4. To study the kinetics of decomposition of the complex formed between sodium sulphide and sodium nitro prusside.
5. To study the inversion of cone sugar in presence of HCl and H_2SO_4 and hence determine the relative strength of the acids.
6. To investigate the autocatalytic reaction between potassium permanganate and oxalic acid.

B Experiments based on spectrophotometry

1. To determine the composition of binary mixture containing $\text{K}_2\text{Cr}_2\text{O}_7$ and KMnO_4 using a spectrophotometer.
2. Test the validity of Bear-Lambert's law and determine the concentration of Glucose solution.
3. To determine the concentration of Metal ions by spectrophotometric titration with EDTA (Copper, Nickel and iron)
4. Determination of ionisation constant of bromophenol blue.
5. To determine phosphate concentration in a soft drink.

C. Green methods (at least one from extraction, synthesis and analysis)

Project & Seminar

The project work should be allotted by a committee constituted at the institute level in the beginning of the semester III. The project should be based on syllabus / local problem / industry / institution. The project should have interdisciplinary approach. The presentation should be in front of a panel and a proper record with geotagged photographs should be maintained.

Books Suggested:

1. Inorganic Experiments, J. Derek Woollins, VCH.
2. Microscale Inorganic Chemistry, Z. Sqafran, R.M Pike and M.M. Singh, Wiley.
3. Practical Inorganic Chemistry, G. Marr and B. W. Rockelt, Van Nostrand.
4. The Systematic Identification of Organic Compounds, R.L Shriner and D.Y. Cutin.
5. Semimicro Qualitative Organic Analysis, N.D. Cheronis, J.B. Entriandin and E.M. Hodnett.
6. Experimental Organic Chemistry, M.P. Doyle and W.S. Mungall.

7. Small Scale Organic Preparations, P.J. Hill.
8. Organometallic Synthesis, J.J. Fisch and R.B. King, Academic.
9. Experimental Physical Chemistry, D.P. Shoemaker, C.W. Garland and J.W. Niber, McGrawHill Interscience.
10. Findlay's Practical Physical Chemistry, revised B.P. Levitt, Longman.
11. Experiments in Physical Chemistry, J.C. Ghosh, Bharti Bhavan.
12. Green Chemistry : An experimental study, R.K. Sharma, N. Bhojak, I.T. Sidhwani and M.K. Choudhary

Semester 3

ELECTIVE PAPERS

Group-D

PRACTICAL PAPER : LC-5-D

CHEMISTRY LAB 5D

Time : 7 Hours

Max. Marks :50 (40 for external 10 for internal)

A Analysis & Determinations

- (i) Determination of very weak acid eg. Vaniline, Isovaline, phenolic compounds etc.) using base (e.g. Lithium hydroxide, barium hydroxide etc.)
- (ii) Study of Precipitation and/Complex formation reaction by drawing titration curve eg. silver salt with lithium chloride, ammonium sulphate with barium acetate, etc.
- (iii) Determination of cations Iron (II) as or anions eg- chloride, dihydrogen phosphate.
- (iv) Determination of free acid in solution of metal salt (e.g. sulphuric acid/in aluminium sulphate, Perchloric acid in uranyl perchlorate)

B Potentiometric/pH Metric method:-

- (i) Determinations of metal-ions, eg. Iron (ii), Copper (ii), Chromate (ii), Manganese (ii) in pyrolusite/steel etc.
- (ii) Determination of metal-ion eg. Calcium (II), Nickel (II) Cobalt (II), Zinc (II) etc.

C. Primary information / experimentations on Indian pharmacopoeia, Ayurvedic pharmacopoeia, BIS methods and ISO methods

Spotting

In spotting there should be 5 spots related with instruments and techniques as per syllabus ; time of spotting is 20 minutes.

IKS : Applied Chemical Science / Technology in Indian Knowledge system

Semester 3

ELECTIVE PAPERS

Group-D

PRACTICAL PAPER : LC-6-D

CHEMISTRY LAB 6D

Time : 7 Hours

Max. Marks :50 (40 for external 10 for internal)

ANALYTICAL CHEMISTRY

A Chromatographic Separation

- (i) Separation of Zinc(II) & Magnesium (II) on an Ion exchanger.
- (ii) Separation of chloride & bromide on an Ion exchanger.
- (iii) Separation & recovery of dyes (eg. bromophenol blue, Congo red, phenol red) using TLC.
- (iv) Separation of artificial colorant in confectionery / pickles / sauces etc. by TLC
- (v) Separation of Chlorophylls

B Solvent Extraction:

- (i) Separation & determination of Copper (II) as diethyldithio carbamate complex.
- (ii) Separation & Determination of Copper (II) as Neocuproin complex.
- (iii) Separation & determination of Iron (II) as 8-hydroxy quinolate.

C Spectrophotometric Determination.

- (i) Determination of Boron/Chromium/Titanium/tungsten in steel.
- (ii) Simultaneous determination- Chromium (II) & Manganese (II).
- (iii) Determination of active constituents in a medicine by derivative spectroscopy e.g. two drugs pseudoephedrine hydrochloride and teriprolidine hydrochloride in "Actified" a medical preparation.
- (iv) Determination of cholesterol.
- (v) Determination of ingredients in soda water etc.

Green methods (at least one from extraction, synthesis and analysis)

Project & Seminar

The project work should be allotted by a committee constituted at the institute level in the beginning of the semester III. The project should be based on syllabus / local problem / industry / institution. The project should have interdisciplinary approach. The presentation should be in front of a panel and a proper record with geotagged photographs should be maintained.

M.Sc. (FINAL) CHEMISTRY,

Semester 4

GENERAL PAPER CC-13

ADVANCES IN SPECTROSCOPY AND PHOTO CHEMISTRY

Time : 3 Hours

Max. Marks :50 (40 for external 10 for internal)

Unit-I

Mossbauer spectroscopy : Basic principles, spectral parameters and spectrum display. Application of the technique to the studies of (1) bonding and structures of Fe^{+2} and Fe^{+3} compounds including those of intermediate spin, (2) 12 Sn and Sn^{+4} compounds - nature of M-L bond, coordination number, structure and (3) detection of oxidation state and in equivalent MB atoms.

Unit-II

Electron Spin Resonance Spectroscopy : Hyperfine coupling, spin polarization for atoms and transition metal ions, spin-orbit coupling and significance of g-tensors, application to transition metal complexes (having one unpaired electron) including biological systems and to inorganic free radicals such as PH_4^+ , F_2^- and $[\text{BH}_3]$

Unit-III

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

(b) Determination of Reaction Mechanism : Classification, rate constants and life times of reactive energy state- determination of rate constants of reactions. Effect of light intensity on the rate of photochemical reactions. Types of photochemical reactions-photo dissociation, gas phase photolysis.

Unit IV

(a) Photochemistry of Carbonyl compounds: Intramolecular reactions of carbonyl compounds-saturated, cyclic and acyclic β,γ - unsaturated and α,β - unsaturated compounds, Cyclohexadienones.

Intermolecular cycloaddition reactions-determinations and oxetane formation.

(b) Photochemistry of Alkenes : Intra molecular reactions of olefinic bond geometrical isomerism, cyclisation reactions, rearrangement 1,4, and 1,5 diens.

Unit-V

(a) Photochemistry of Aromatic Compounds : Isomerisations, additions and substitutions.

(b) Miscellaneous Photochemical Reactions : Photo- Fries reactions of anilides. Photo-fries rearrangement.

Barton reaction. Singlet molecular oxygen reactions. Photochemical formation of smog. Photodegradation of polymers. Photochemistry of vision.

Book Suggested :

- 1- Fundamentals of Photochemistry, K.K. Rohtagi- Mukerji, Wiley- Eastern.
- 2- Essentials of Molecular Photochemistry, A. Gilbert and J. baggott, Blackwell Scientific Publication.
- 3- Molecular Photochemistry, N.J. Turro, W.A. Bejamin.
- 4- Introductory Photochemistry, A Cox and T. Camp, Mc- Graw Hill.
- 5- Photochemistry, R.P. Kundall and A. Gillbert, Thomson Nelson.
- 6- Organic Photochemistry, J. Coxon and B. Halton, Cambridge University press.
- 7- Solid State chemistry and its Applications, A.R. West Plenum.
- 8- Principles of the Solid, H.V. Keer, Wiley eastern.

Semester 4

GENERAL PAPER-CC 14

CHEMICAL BIOLOGY AND COMPUTER IN CHEMISTRY

Time : 3 Hours

Max. Marks :50 (40 for external 10 for internal)

UNIT-I

- (a) Metal Ions in Biological Systems :** Essential and trace metals.
- (b) Na⁺/K⁺ Pump** Role of metals ions in biological processes
- (c) Bioenergetics and ATP Cycle:** DNA Polymerisation, glucose storage, metal complexes in transmission of energy, chlorophylls photo system I and photo system II in cleavage of water. Model systems.

Unit II

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

Electron Transfer in Biology : Structure and function of metalloproteins in electron transport process – cytochromes and iron-sulphur proteins, synthetic models.

Unit-III

Biotechnological Application of Enzymes : Large- Scale production and purification of enzymes, techniques and methods of immobilization of enzymes, effect of immobilization of enzyme activity, application of immobilized enzymes. Use of enzymes in food and drink industry-brewing and cheese making syrups from corn starch enzymes as targets for drug design. Clinical uses of enzymes, enzyme therapy, enzymes and recombinant DNA technology.

Unit-IV

Programming in Chemistry : Development of small computer codes involving simple formulae in chemistry, such as Van der Waal equation, PH titration, kinetics, radioactive decay (half life and average life) determination of Normality. Molarity and Molality of Solutions. Evaluation of electronegativity of an atom and lattice energy and ionic radii from experimental data. Linear simultaneous equations to solve secular equations within the Huckel theory. Elementary structural features such as bond lengths. Bond angles, dihedral angles etc. of molecules. Extracted use of computer programmes from data base such as Cambridge Data Base.

Unit-V

Use of Computers Programmes : Operations of PC. Data Processing. Running of standard programs and packages such as MS WORD, MS EX-CEL-special emphasis on calculations and chart formation. X-Y plot. Simpson's Numerical Integration method. Programmes with data preferably from physical chemistry laboratory. Introduction of working of any one of the packages such as LOTUS/EXCEL/FOXPROM/MOPAC and Word Processing software such as WORDSTAR/MS WORD.

Books Suggested:-

- 1- Principles of Bioinorganic Chemistry S.J. Lippard and J.M. Berg, University Science Books.
- 2- Bioinorganic chemistry, I Bertini, H.B. Gray, S.J. Lippard and J.S. Valentine, University science books.
- 3- Inorganic Biochemistry vols I and II G.L. Eichhorn Elsevier.
- 4- Progress in Inorganic Chemistry, Vols 19 and 38ed, J.J. Luippard, Wiley.
- 5- Bioorganic chemistry : A Chemical Approach to Enzyme Action, Heeeeermann Dugas and C. Penny, Springerverlag.
- 6- Understanding Enzymes, Trevor Palmer, Prentice Hall.
- 7- Enzyme Chemistry : Impact and Applications, Ed. Collin J. Sucking Chapman and Hall.
- 8- Fundamental of Enzymology, NC, Price and L. Stevens Oxford, University Press.
- 9- Immobilized Enzymes An Introduction and Application in Biotechnology, Miehael D. Trevan, John wiley.
- 10- Enzymatic Reaction Mechanisms, C. Waish, W.H. Freeman.
- 11- Enzyme Structure and Mechanism, A Fersht, W.H. Freeman.
- 12- Biochemistry : The chemical Reactions of Living Cells, D.E. Metzler, Academic Press.
- 13- Enzyme Mechanisms Ed. M.L. Page and A. Williams, Royal Society of chemistry.
- 14- Principle of Biochemistry, A.L. Lehinger, Worth Publishers.
- 15- Biochemistry . L. Stryer. W.H. Freeman.
- 16- Biochemistry, J. David Rawn, Neil Patterson.

- 17- Biochemistry, Voet and Voet, John Wiley.
- 18- Outline of Biochemistry, E.E. Conn and P.K. Stumpe, John Wiley.
- 19- Bioorganic Chemistry : A Chemical Approach to Enzyme Action. H. Dugas and C. Penny, Springer-Verlag.
- 20- Computational Chemistry, A.C. Norris, John Wiley.
- 21- Computer Programming in FORTRAN 77, R Rajasthan, Prentice Hall.

Semester 4

ELECTIVE PAPERS

Group-A

PAPER : CC-15-A

ADVANCED INORGANIC CHEMISTRY Part 2

Time : 3 Hours

Max. Marks :50 (40 for external 10 for internal)

Unit-I

Compounds of Transition Metal- Carbon Multiple Bonds : Alkylidenes, alkylidynes, low valent carbenes and carbenes- synthesis, nature of bond, structural characteristics, nucleophilic reactions on the ligands, role in organic synthesis.

Unit-II

Metal in Medicine : Metal deficiency and disease, toxic effects of metals, metals used for diagnosis and chemotherapy with particular reference to anticancer drugs

Unit-III

Fluxional organometallic compounds: Fluxionality and dynamic equilibria in compounds such as η^2 – η^3 allyl and dienyl complexes

Unit-IV

Metal storage transport and biomineralisation: Ferritin ,Transferrin and siderophores.

Unit-V

Advanced Supramolecular Chemistry :

- (a) Supramolecular reactivity and catalysis.
- (b) Transport processes and carriage design.
- (c) Supramolecular devices supramolecular photochemistry, supramolecular electronic, ionic and switching devices.

Books Suggested :

- 1- Principles and application of Organotransition Metal chemistry, J.P. Collaman, L.S Heddus, J.R. Norton and R.G. Finke, University Science books.
- 2- The Organometallic chemistry of the Transition Metals, R.H. Crabtree John Wiley.
- 3- Metallo- Organic Chemistry, A.J. Pearson, Wiley.
- 4- Organometallic Chemistry, R.C. Mehrotra and A. Singh, New Agee International.
- 5- Principles of Bioinorganic Chemistry, S.J. Lippard and J.M. Berg, University Science Books.
- 6- Bioinorganic Biochemistry, I. Bertini, H.B. Gray, S.J. Valentine, University Science Books.
- 7- Inorganic Biochemistry vols I and II G.L. Eichhorn Elsevier.
- 8- Progress in Inorganic Chemistry, Vols 18 and 38 ed. J.J. Lippard, wiley.
- 9- Supramolecular Chemistry, J.M. Lehn, VCH

Semester 4

ELECTIVE PAPERS

Group-A

PAPER : CC-16-A

CERAMICS AND ADVANCED POLYMERS

Time : 3 Hours

Max. Marks :50 (40 for external 10 for internal)

Unit-I

Ceramics Technology :

- (a) Description and classification of various minerals based on their chemical compositions, Physical properties and occurrence.
- (b) Study in detail of raw materials used in glass, Refractories, White wares, Potteries and Cement

Unit-II

Characterization of Ceramics

Chemical characteristic of raw materials of alkali and alkaline earth elements, Silica, Silicates, Alumina, Aluminates, Titania, Zirconia and zircon, Chromatography : Introduction, Paper and thin layer chromatography, Liquid chromatography, Types of liquid chromatography, Column and detection systems. Differential thermal analysis (DTA) and thermo gravimetric analysis (TGA) with suitable examples.

Unit-III

Polymer characterization : polydispersion – average molecular weight concept. Number, weight and viscosity average molecular weights Polydispersity and molecular weight distribution. The practical significance of molecular weight measurement of molecular weights. End-group, viscosity light scattering,

osmotic and ultracentrifugation methods, X-ray diffraction study Microscopy. Thermal analysis and physical testing – tensile strength. Fatigue, impact. Tear resistance. Hardness and abrasion resistance.

Polymer processing : Plastic elastomers and fibers. Compounding processing techniques calendaring, die casting rotational casting, film casting, injection molding, blow molding, extrusion molding, thermoforming, foaming, reinforcing and fiber spinning.

Unit IV

Structure and Properties : Morphology and order in crystalline polymers –configurations of polymer chains. Crystal structure of polymers. Morphology of crystalline polymers , strain induced morphology, crystallization and melting polymer structure and physical properties – crystalline melting point. T_m Melting points of homogeneous series, effect of chain flexibility and other steric factors, entropy and heat of fusion. The glass Transition temperature, T_g - Relationship between T_m and T_g . Effects of molecular weight diluents, chemical structure chain topology, branching and cross linking property requirements and polymer utilization.

Unit-V

Commercial Polymers :

Polyethylene, polyvinyl chloride polyamides , polyesters, phenolic resins, epoxy resins and silicone polymers. Functional polymers- fire retarding polymers and electrically conducting polymers Biomedical polymers- contact lens. Dental polymers, artificial heart, kidney, skin and blood cells.

Books Suggested :

- 1- Concepts of inorganic photochemistry, A.W. Adamson and P.D. Fleischauer, Wiley.
- 2- Inorganic Photochemistry, J. Chem. Educ. Vol. 60, No10, 1983
- 3- Progress in inorganic chemistry, vol 30 ed, S.J. Lippard Wiley.
- 4- Coordination Chem. Revs. 1981, vol39, 121, 131, 1975, 15, 321, 1970 97, 113
- 5- Photochemistry of Coordination Compounds, V. Balzani and V. Carassiti Academic press.
- 6- Elements of inorganic photochemistry, G.J. Willey.
- 7- Textbook of polymer Science, F.W. Lamba, Prentice Hall
- 8- Physical and Chemistry of polymers, J.M.G. Cowie, Blackies Academic and Professional.
- 9- Functional monomers and polymers, K. Takemoto, Y. Inaki and R.M. Otanbrite.
- 10- Contemporary polymers Chemistry, H.R. Alcock and F.W. Lambe, Prentice Hall.
- 11- Polymers of science V.R. Gowarikar, N.V. Vuswanathan and J. Sreedhar Wiley- Eastern.

ELECTIVE PAPERS

Group-B

PAPER : CC-15-B

ORGANIC SYNTHESIS Part 2

Time : 3 Hours

Max. Marks :50 (40 for external 10 for internal)

Unit-I

Disconnection Approach: An Introduction to synthons and synthetic equivalents, disconnection approach, functional group inter-conversions, the importance of the order of events in organic synthesis, one group- C-X and two group C-X disconnections, chemoselectivity reversal of polarity, cyclisation reactions, amine synthesis.

Unit-II

One groups C-C disconnections : Alcohols and carbonyl compounds, regioselectivity, alkene synthesis, uses of acetylenes and aliphatic nitro compounds in organic synthesis.

(b) Two group C-C disconnections : Diels – Alder reaction, 1-3 difunctionalised compounds, alpha & beta unsaturated carbonyl compounds, control in carbonyl condensations, 1,5- difunctionalised compounds, Micheal addition and Robinson annulation.

Unit III

Ring Synthesis : Saturated heterocycles, synthesis of 3-,4-, 5- and 6-membered rings aromatic heterocycles in organic synthesis.

Unit IV

Protecting groups : Principles of protection of alcohol, amine, carbonyl and carboxyl groups.

Unit-V

Synthesis of Some Complex Molecules : Camphor, Longifoline, cortisone, reserpine, vitamin D, Juvalbione, Aphidicolin and Fredericamycin A.

Books Suggested :

- 1- Modern Synthetic Reactions, H.Q. House, W.A. Benjamin.
- 2- Some modern Methods in organic synthesis, W, Carruthers, Cambridge University press.
- 3- Advanced Organic Chemistry reactions mechanisms and structure J March John Wiley.
- 4- Principles of Organic Synthesis, RoC Norman and J.M. Coxon, Blackie Academic & Professional.
- 5- Advanced organic chemistry Part-B, F.A. Carey and R.J. Sundberg Plenum press.
- 6- Rodd's chemistry carbon compounds, ed S. Coffey, Elsevier.
- 7- Designing organic synthesis S Warren Wiley.
- 8- Organic synthesis – concepts, methods and starting materials J Furrow and G. Penzlin, VCH.

- 9- Some modern methods of organic synthesis W.E. Carruthers Cambridge Univ. Press.
- 10- Modern synthesis reactions, H.Q. House W.A.A. Benjamin.
- 11- Advanced organic chemistry reactions, Mechanisms and structure, March Willy
- 12- Principle of organic synthesis, R. H. Norman and J.M. Cozon, Blackie academic & professional.
- 13- Advanced organic chemistry Part-B.F.A. Carey and R.J. Sundberg. Plenum press.

Semester 4

ELECTIVE PAPERS

Group-B

PAPER : CC-16-B

HETEROCYCLICS AND NATURAL PRODUCTS Part 2

Time : 3 Hours

Max. Marks :50 (40 for external 10 for internal)

Unit-I

Five membered heterocycles with one & two heteroatoms : Synthesis & reactions of Pyrrole, thiophene, furan, pyrazole, imidazole, oxazole and thiazole.

Terpenoids and Carotenoids : Classification, nomenclature, occurrence, isolation, general methods of structure determination, isoprene rule.

Unit-II

Structure determination, stereochemistry, biosynthesis and synthesis of the following representative molecules : Citral, Geraniol, α -terpineol, Menthol, Zingiberene, Santonin and β -carotene.

Unit-III

Alkaloids : Definition, nomenclature and physiological action, occurrence isolation, general methods of structure elucidation, degradation classification based on nitrogen heterocyclic ring, role of alkaloids in plants.

Structure, stereochemistry, synthesis and biosynthesis of the following : Ephedrine, (+)-coniine, nicotine, atropine quinine and morphine.

Unit IV

Porphyrins : structure and synthesis of hemoglobin and chlorophyll.

Plant pigment : Occurrence, nomenclature and general methods of structure determination, isolation and synthesis of quercetin and myrcetin.

Unit-V

Steroids : Occurrence, nomenclature, basic skeleton, Diel's hydrocarbon and stereochemistry. Isolation, structure determination and synthesis of cholesterol, bile acids, androsterone, estrone, estrone, progesterone, aldosterone. Biosynthesis of steroids.

Books Suggested :

- 1- Heterocyclic chemistry Vol, 1-3, R.R. Gupta, M. Kumar and V. Gupta springer Verlag.
- 2- The Chemistry of Heterocycles, T. Eicher and S. Hauptmann, thieme.
- 3- Heterocyclic chemistry, J.A. Joule, K. Mills and G.F. Smith, Chapamn and Hall.
- 4- Heterocyclic Chemistry, T.L. Gilchrist, Longman Scientific Technial.
- 5- Contemporary Heterocyclic compounds, R.M. Acheson, John Wiley.
- 6- An introductoni to the Heterocyclic compounds R.M. Acheson, John Wiley.
- 7- Compreshensive Heterocyclic Chemisty, A.R. Kartizky and C.w. Reeds, edg. Pergamon Press.
- 8- Natural Poducts : chemistry and Biological Singificance, J Mann, R.S. Davidson, J.B. Hobbs, D.V. Banthrope and J.b. Harborn, Longman Essex.
- 9- Organic Chemistry, Vol2, I.L. Finar Elbs.
- 10- Stereoselective synthesis : A practical Approach, M. Nogradi, BCH.
- 11- Rodd's Chemistry of Carbon Compounds, Ed. S. Coffey, Elsevier.
- 12- Chemistry, biological and Pharmacological Properties of Medicainal Plants from the Americas, Ed Kurt Hostettmann, M.P Gupta and A. Marston, Harwood Academic Publishers.
- 13- Introduction to Flavonoids, B.A. Bohm, Harwood, Academic Publishers.
- 14- New trens in natural products chemistry Atta- Ur Rahman and Mi.L. choudhary, Harwood Academic Publishers.
- 15- Insecticides of Natural Origin Sukhdev, Harwood Academic Publishers.

Semester 4

ELECTIVE PAPERS

Group-C

PAPER : CC-15-C

RECENT TRENDS IN PHYSICAL CHEMISTRY

Time : 3 Hours

Max. Marks :50 (40 for external 10 for internal)

Unit-I

Concept in molecular orbital (MO) and Valence Bond (VB) Theory: Introduction to Huckel Molecular orbital (MO) method as a means to explain modern theoretical methods. Advanced techniques in PMO and FMO theory. Molecular mechanics, semi empirical methods and ab initio and density functional methods. Scope and limitations of several computational programmes.

Unit-II

Quantitatives MO theory- Huckel molecular orbital (HMO) method as applied to ethane, allyl and butadiene. Qualitative Mo theory- ionization potential. Electron affinities. MO energy levels. Orbital symmetry orbital interaction diagrams. MO of simple organic systems such as ethene, allyl, butadiene, methane and methyl group conjugation and hyperconjugation. Aromaticity. Valene bond (VB) configuration mixing diagrams. Relationship between VB configuration mixing and resonance theory

reaction profiles. Potential energy diagrams. Curve- crossing model-nature of activation barrier in chemical reactions.

Unit III

Theory of liquid : Theory of liquids partition function method or model approach single cell models communal energy and entropy. LTD model, significant structure model.

General properties of Liquids-

(i) Liquids as dense gases, liquids as disordered solids, some thermodynamics relations, internal pressure and its significance in liquids. Equation of state, critical constants. Different types of intermolecular forces in liquids, different potential functions for liquids, additivity of pair potential approximation.

(ii) A classical partial function for liquids, correspondence principle, configuration integral configuration properties.

Unit IV

Supercooled and Ionic Liquids : Super cooled and ionic liquids theories of transport properties : non Arrheniusbehaviour of transport properties non Arrheniusbehaviour of transport properties cohen-trunbull free volume model, configurational entropy model, macedolito-vitz hybrid model, glass transition in super cooled liquids.

Unit V

SOLID STATE CHEMISTRY

Metals, insulators and semiconductors, electronic structure of solids, band theory, band structure of metals, insulators and semiconductors, intrinsic and extrinsic semiconductors, doping semiconductors, p-n junctions and superconductors.

Book Suggested :

- 1- Molecular Mechanics, U burkert and N.L. Allinger, ACS Monograph 177, 1982.
- 2- Organic Chemists' book of orbitals. L Salem and W.L. Jorgensen, Academic Press.
- 3- Mechanism and Theory in Organic Chemistry, T.H. Lowry and K.C. Richardson, Harper and Row.
- 4- Introduction to Theroretical Organic Chemistry and Molecular. Modeling, W.B. Smith, VCH Weinheim.
- 5- Physical Organic Chemistry, N.S. Lssacs, ELBS/Longman.
- 6- Supramolecular Chemistry, Concepts and Persopective, JM Lehn, VCH.

- 7- The physical Basis of Organic Chemistry, H. Haskill, Oxford University Press.
- 8- An introduction to Liquid State, P.A. Egelstaff, Academic Press.
- 9- The Dynamic State, A.F.M. Barton, Longman.
- 10- Introduction to Statistical Thermodynamics T.L. Hill Addison Wiley.
- 11- The Liquid State, J.A. Pryde.
- 12- Significant Liquid Structures, H. Eyring and M.S. John

Semester 4

ELECTIVE PAPERS

Group-C

PAPER : CC-16-C

COMPUTATIONAL CHEMISTRY

Time : 3 Hours

Max. Marks :50 (40 for external 10 for internal)

Unit-I

Fortran / Programming and Numerical Methods : Advanced programming features of FORTRAN /C. Basic theory, discussion of algorithms and errors for the following numerical methods. Examples from chemistry should be selected for illustrating the methods.

Solution Equations : Bisection, regular falsi, Newton- Raphson and related methods for solving polynomial and transcendental equations convergence. Errors and Ill- conditioning

Linear Simultaneous Equations : Gaussian elimination, Gauss-Seidel method Gauss-Jordan method. Pivoting strategy. Errors and ill conditioning.

Eigen values and Matrix Diagonalization : Jacobi and Householder methods, analysis or errors.

Unit-II

Interpolation : Newton forward and backward difference, central differenced formulae. Lagrange and Hermite interpolation. polynomial wiggle problem.

Numerical differentiation : Solutions of simple differential equation by Taylor series and Runge- Kutta methods.

Numerical integration : Newton- Cotes formulae, Romberg integration, errors in integration formulae.

(vii) The students should develop computer programs for some of the above numerical methods.

Unit-III

Running of Advanced scientific Packages : The students are expected to get hands on experience of running a few selected advanced level scientific software package after a brief introduction to the basic theory and methodology. Ab initio quantum chemical packages such as GAUSSIAN/ GAMES with carefully designed exercise for illustrating various features of the packages. Semi- empirical / Dynamic / simulation packages such as MOPAC, CHARM, AMBER, QUANTA etc. Basic ideas on structure activity relating drug and catalysis design etc.

Unit-IV

Computer Experiments : Computer experiments using quantum chemistry – software packages such as GAUSSIAN./ GAMESS / MOPAC and modeling software e.g. MM2/AMBER/CHARM etc.

Unit-V

Theoretical and Computational Treatment of Atoms and Molecules, Hartree-Fock theory.

Review of the principles of quantum mechanics, Born- Oppenheimer approximation. Slater-Condon rules, Hartree-Fock equation, Koopmans and Brillouin theories, Roothaan equation, Gaussian basis sets.

Book Suggested :

- 1- Computational Chemistry, A.C. Norris, John Wiley.
- 2- Computer Programming in FORTRAN 77, R Rajasthan, Prentice Hall.
- 3- Numerical Analysis, CE. Frogberg, Macmillan.
- 4- Numerical Analysis-A Practical Approach, M.J. Merson, John Wiley.
- 5- Numerical Methods for scientists and Engineers H.M. Antia Tat McGraw Hill.
- 6- Modern Quantum Chemistry N.S. Ostlund and A. Szabo, McGraw Hill.
- 7- Methods of Molecular Quantum Mechanics, R. Mcweeny and B.T. Sutcliffe, Academic Press.
- 8- Density Functional Theory of Atoms and Molecules, R.G. Parr and W Yang, Oxford.
- 9- Exploring Chemistry with Electron Structure Methods, J.B. Foresman and E. Frisch Gaussian Inc.
- 10- Semi-Empirical MO Theory, J. Pople and D.L. Beveridge.

Semester 4

ELECTIVE PAPERS

Group-D

PAPER : CC-15-D

ANALYTICAL CHEMISTRY Part 2

Time : 3 Hours

Max. Marks :50 (40 for external 10 for internal)

UNIT-I

UV-Vis Spectrophotometry:- Theory, instrumentation, experimental technique for determination, differential and derivative spectroscopy, photometric titrations.

UNIT-II

Fluorescence & Phosphorescence Spectrophotometry :Basic principles, instrumentation, experimental technique and important application.

Fluorimetry, Nephelometry & Turbidimetry: Basic principles, instrumentations, experimental technique & important applications.

UNIT-III

Atomic Absorption and Flame Emission Spectroscopy(AAS &FES): Elementry theory, Instrumentation for atomic absorption & Reame emission spectroscopy, experimental technique and important applications. Comparison of AAS& FES.

UNIT-IV

Chromatography: Basic principles, Instrumentation, experimental technique and important application of following-

- (a) Thin layer chromatography(TCL), paper, column, Ion-Exchange chromatography
- (b) Gas Chromatography (GC), Gas Liquid Chromatography (GLC), High performance liquid chromatography (HPLC).

UNIT-V

Ceramic analysis and Instrumentation

- (a) Description and classification of various minerals based on their chemical compositions, Physical properties and occurrence.
- (b) Study in detail of raw materials used in glass, Refractories, White wares, Potteries and Cement
- (c) Chemical characteristic of raw materials of alkali and alkaline earth elements, Silica, Silicates, Alumina, Aluminates, Titania, Zirconia and and zircon, Chromatography : Introduction, Paper and thin layer chromatography, Liquid chromatography, Types of liquid chromatography, Column and detection systems. Differential thermal analysis (DTA) and thermo gravimetric analysis (TGA) with suitable examples.

Books Suggested :

- 1- Analytical Chemistry, G.D. Christian, J. Wiley.
- 2- Fundamentals of Analytical Chemistry, D.A. Skoog,, D.M. Westand F.J. Holler, W.B. Saunders.
- 3- Analytical Chemistry – Principles, J.H. Kennedy, W.B. Saunders.
- 4- Analytical chemistry – Principles and techniques, LG. Hargis, Prentice Hall.
- 5- Principles of Instrumental Analysis, D.A. Skoog, J.L. Loary, W.B. Saunders.
- 6- Principles of Instrumental Analysis, D.A. Skoog, W.B. Saunders.
- 7- Quantitative Analysis, R.A. Day, Jr. and A.L. Underwood Prentice Hall.
- 8- Basic Concepts of Analytical Chemistry, S.M. Kholkar, Wiley Eatern.
- 9- Handbook of Instrumental Techniques for Analytical Chemistry, F. Settle Prentice Hall.

Semester 4

ELECTIVE PAPERS

Group-D

PAPER : CC-16-D

APPLIED ANALYTICAL CHEMISTRY Part 2

Time : 3 Hours

Max. Marks :50 (40 for external 10 for internal)

Unit-I

Environmental Analysis : Metallic and non-metallic pollutants, Cr, Hg, Pb,Cd,Cu,As etc. Their physiological manifestation, source, analysis and control of inorganic compounds. Chemistry of Air pollutants, Characterization. Source, methods of analysis of air pollutants ; CO,CO₂, NOX,NH₃,H₂S,SO₂,etc. Monitoring Instruments, Potable and Industrial water, major and minor components, dissolved oxygen(DO) Chemical oxygen demand(COD) Biochemical oxygen demand(BOD) and their measurements and significance in waste water treatments, Threshold odour number.

Unit-II

Industrial waste Water analysis for organic and Inorganic Constituents: Chemistry of odour and its measurements Sewage and sludge analysis. Treatment, disposal and source of phenolic residue, Analytical methods, treatment by using stream. Gas stripping, ion exchange, solvent extraction, oxidation method and microbiological treatment.

Unit-III

Forensic analysis:- Sampling, sample storage, sample dissolution, classification of poisons, Lethal dose, significance of LD 50 and LC 50. Types of drug doses for crime investigations. Special case studies.

Unit-IV

Analysis of dyes and paints: Types of dyes, and their analysis. Composition and analysis of paints, determination of volatile and non-volatile constituents, flash points, separation of pigments, estimation of binders and thinners.

Unit -V

Analysis of oils, fats, soaps and detergents: Introduction to natural fats and oils, Analysis of oils and fats: Softning point, Congent point, Titre point, cloud point, Iodine, Saponification, acid, hydroxyl, R-M and Polenske value, Elaiden test.Introduction to soaps, analysis of soap (saponifiable, unsaponifiable) and for unsaponified matter in soaps, Estimation of free alkali and phenol in soap. Classification of detergents (in Brief): Analysis of active ingredients from detergents (methylene blue and Hyamine-1622 method); Estimation of CMC, Chlorides, total phosphates etc.

Reference Books:

1. F. J. Welcher: Standard methods of Chemical analysis, 6th Ed. Vol. I and II(D. Van Nostard Comp.)
2. I. M. Kolthoff: Treatise on Analytical Chemistry Vol. I & II
3. F. D. Snell: Encyclopedia of industrial Chemical Analysis Vol. 1 to 20 (John Wiley)
4. Riech: Outline of Indutrial Chemistry.

5. K. H. Buchel: Chemistry of Pesticides (John Wiley)
6. Nichollas: Aids to the Analysis of foods and Drugs.
7. A. H. Beckett and J. B. Stanlake; Practical Pharmaceutical Chemistry Vol. I & II (CBS publishers)
8. S. Ranganna: Handbook of analysis and quality control for fruits and vegetable products (McGraw Hill)
9. Ramalu: Analysis of pesticides
10. Bassett, Denney-Jeffer and Mendham, Vogel's Textbook of Quantitative Inorganic Analysis, (5th edition).
11. A.K. De : Standard Methods of Waste and Waste water analysis.
12. S.M. Khopkar, Environmental Chemistry ; Environmental pollution analysis.
13. M.S. Creos and Morr, Environmental Chemical Analysis, American publication (1988)
14. A.K. De, Environmental Chemistry, New Age International publishers. Moghe and
15. Ramteke, Water and waste water analysis : (NEERI)
16. A.C. Stern, Air pollution: Engineering control vol.IV (AP)
17. P.N. Cheremisinoff and R.A. Young, Air Pollution control and Design. Hand Book Vol. I & II (Dekker)
18. B.K. Sharma, Industrial Chemistry.
19. S.P. Mahajan, Pollution Control in Process Industries.
20. R.A. Horne, Chemistry of our Environment.
21. Ruzica and Sary, Substochiometry in Radiochemical Analysis. Pergamon.
22. Ladd and Lee, Radiochemistry.
23. Clerk, Handbook of Radiochemical methods
24. Hillebrand Lhundel, Bright and Hoffiman, Applied Inorganic Analysis, John Wiley.
25. Snell and Biffen, Commercial Methods of Analysis.
26. P.G. Jeffery, Chemical Methods of Rock Analysis, Pergamon.
27. Allan Cury, Irvins Sunshine, Forensic Analysis, Academic Press Publications.
28. Karamer Twig: Quality control for food industry (AVI)
29. G. F. Longonan: the analysis of detergents and detergent products (JW)
30. A. Davidsohn & B. M. Mlwidaky : Synthetic detergents (Book center, Mumbai)
31. Chopra and Kanwar, Analytical Agriculture Chemistry, Kalyani Publishers.
32. Aubert and Pintes, Trace Elements in Soils.
33. Bear, Chemistry of Soil.
34. Hauson, Plant Growth Regulators, Noyes.
35. Tewari SN, Analytical methods in Forensic Toxicology, Selective & Scientific Books, (2019)

Semester 4

ELECTIVE PAPERS

Group-A

PRACTICAL PAPER : LC-7-A

CHEMISTRY LAB 7A

Time : 7 Hours

Max. Marks :50 (40 for external 10 for internal)

A. Flame Photometric / AAS / ICPMS Determinations (Any Three)

- a. Sodium and potassium when present together
- b. Lithium/calcium/barium/strontium.
- c. Cadmium and magnesium in tap water.
- d. Sulphate.
- e. Phosphate.
- f. any other metal ion as per availability.

B. Chromatographic Separations

Separation and identification of the sugars present in the given mixture of glucose, fructose and sucrose by paper chromatography / TLC / HPTLC and determination of R_f Values.

C. Preparation of nanoparticles of metals or metal compounds or Green Preparation of biodiesel / Interdisciplinary Green chemistry experiment

Preparation and characterization of Biodiesel from vegetable oils (Biodiesel may be prepared from different oils, catalysts and determination of their physical properties viz viscosity, surface tension, flash point.

Spotting

In spotting there should be 5 spots related with instruments and techniques as per syllabus ; time of spotting is 20 minutes

IKS : Applied Chemical Science / Technology in Indian Knowledge system

Semester 4

ELECTIVE PAPERS

Group-A

PRACTICAL PAPER : LC-8-A

CHEMISTRY LAB 8A

Time : 7 Hours

Max. Marks :50 (40 for external 10 for internal)

- A. Experiments of AR, VR, Virtual Laboratory, Molecular models related with simple, complex, polymeric inorganic / organic molecules and methods of analysis (At least two) (10% marks in internal as well as in external)
- B. Designing / Fabrication of low cost instruments or techniques / Green audit of campus, town, city etc. (10% marks in internal as well as in external)
- C. Experiments based on Indian Knowledge system in chemical sciences (10% marks in internal as well as in external)
- D. Spotting – this should include at least five major instruments other than glassware, charts etc. (10% marks in internal as well as in external)
- E. Seminar (10% marks in internal as well as in external)
- F. Project work followed by presentation. The project work should be allotted by a committee constituted at institute level in the beginning of the semester IV and a place / space / workstation should be provided to the students by the institution for the completion of project. The presentation should be in front of a panel and a proper record with geotagged photographs should be maintained. (50% marks in internal as well as in external.)

Semester 4

ELECTIVE PAPERS

Group-B

PRACTICAL PAPER : LC-7-B

CHEMISTRY LAB 7B

Time : 7 Hours

Max. Marks :50 (40 for external 10 for internal)

A. Analysis

Identification of organic compounds by the analysis of their spectral data (UV, IR, PMR, CMR & MS)

B. Spectrophotometric (UV/VIS) Estimations (Any Three)

- | | |
|------------------|----------------|
| 1. Amino acids | 2. Proteins |
| 3. Carbohydrates | 4. Cholesterol |
| 5. Ascorbic acid | 6. Aspirin |
| 7. Caffeins | |

C. Green Preparation of biodiesel / Interdisciplinary Green chemistry experiment

Preparation and characterization of Biodiesel from vegetable oils (Biodiesel may be prepared from different oils, catalysts and determination of their physical properties viz viscosity, surface tension, flash point)

Spotting

In spotting there should be 5 spots related with instruments and techniques as per syllabus ; time of spotting is 20 minutes

IKS : Applied Chemical Science / Technology in Indian Knowledge system

Semester 4

ELECTIVE PAPERS

Group-B

PRACTICAL PAPER : LC-8-B

CHEMISTRY LAB 8B

Time : 7 Hours

Max. Marks :50 (40 for external 10 for internal)

- A. Experiments of AR, VR, Virtual Laboratory, Molecular models related with simple, complex, polymeric inorganic / organic molecules and methods of analysis (At least two) (10% marks in internal as well as in external)
- B. Designing / Fabrication of low cost instruments or techniques / Green audit of campus, town, city etc. (10% marks in internal as well as in external)
- C. Experiments based on Indian Knowledge system in chemical sciences (10% marks in internal as well as in external)
- D. Spotting – this should include at least five major instruments other than glassware, charts etc. (10% marks in internal as well as in external)
- E. Seminar (10% marks in internal as well as in external)
- F. Project work followed by presentation. The project work should be allotted by a committee constituted at institute level in the beginning of the semester IV and a place / space / workstation should be provided to the students by the institution for the completion of project. The presentation should be in front of a panel and a proper record with geotagged photographs should be maintained. (50% marks in internal as well as in external.)

Semester 4

ELECTIVE PAPERS

Group-C

PRACTICAL PAPER : LC-7-C

CHEMISTRY LAB 7C

Time : 7 Hours

Max. Marks :50 (40 for external 10 for internal)

A. Advanced Experiments

1. Determination of partial molar volume of solute (KCl) and solvent in a binary mixture.
2. Determination of the temperature dependence of the solubility of a compound in two solvents having similar intermolecular interactions (benzoic acid in water and in DMSO water mixture) and calculate the partial molar heat of solution.
3. Determination of p_{Ka} of an indicator (methyl red) in (i) aqueous and (b) micellar media.
4. Characterization of the complexes by electronic and IR spectral data.
5. Estimation of Pb²⁺ and Cd²⁺/Zn²⁺ and Ni²⁺ by polarography.
6. Determination of dissolved oxygen in aqueous solution of organic solvents.
7. Experiments related with computational and virtual chemistry may be designed and performed.

B Experiments based on Electronics:-

This lab course will have theory as well as practical and the lectures shall be delivered during lab hours.

Basic Electronics:

Notations used in the electronic circuit, study of electronic compounds and colour codes, conversion of chemical quantities into electronic quantities transducer, illustration with electrodes, thermocouples and thermistors.

Passive components;

Resistors capacitors and inductors with some emphasis on solid state properties of materials. Network theorems of resistors Thevenin's theorem super position theorem loop analysis, R.C. circuits in NMR Spectroscopy, Mossbauer spectroscopy cyclic voltammetry and in power supplies as circuits.

Active Components :

Introduction to ordinary diodes and Zener diodes with some emphasis on p-n junction as a solid state property. Use of diodes as rectifiers clipping and clamping circuits power supplies.

Transistor:

An extension of p-n junction of pnp and npn transistors Characteristics of transistors ,hybrid parameter, transistor circuits as amplifiers, high impedance (preamplifier) circuits, darlington pairs differential amplifiers.

Operational Amplifiers

Ideal Characteristics; inverter, summer, integrator, differentiator, voltage follower, illustrative use of operational amplifiers. Introduction to Fourier transformation in instrumentation

List of Experiments in Electronics

(Do at least five experiments from this section)

1. (a) To plot the diode characteristics and find its dynamic resistance and cut in voltage.
(b) To plot the characteristics of a transistor used as a diode and compare the results with those of (a)
2. To implement a diode clipper circuit for the given transfer characteristics and verify the wave form.

3. To implement a diode damper circuit which damps the positive peak of the input voltage to (a) Zero voltage and (b) a given voltage. Verify the performance.
4. (a) To Plot the characteristics of an NPN transistor in CE configuration, (b) To find the h-parameter of the transistor from the characteristics.
5. (a) To plot the characteristics of an NPN transistor in CB configuration. (b) To find the h-parameter of the transistor from the characteristics and compare it with the results of experiment No. 6
6. (a) To plot the drain and transfer characteristics of JEET in CS configuration, (b) To find out the pinch off voltage, maximum drain to source saturation current and the trans conductance.
7. To obtain the frequency response of an RC coupled amplifier and estimate the bandwidth.
8. (a) To Plot the characteristics of Zener diode and find its dynamic resistance under reverse biased condition
(b) To use zener diode for a. voltage regulation
(i) Plot the line regulation curve,
(ii) Plot the low regulation curve.
9. (a) To wire a half wave Rectifier circuit using diode and measure the rms voltage, dc voltage and to find Ripple factor.
(b) To study the performance of Half wave and full wave doubler circuits.
10. To plot characteristics of UJT and find the peak voltage, peak current and valley voltage and use as a relaxation.

Note: A Sheet containing 20 questions/diagrams/circuits will be provided to the students to reply. These questions based on basic electronics will cover both theory and practicals as provided in the syllabi. They will be of objective type for duration of 20 minutes with maximum scoring of 10 marks.

B. Interdisciplinary Green chemistry experiment

Preparation and characterization of Biodiesel from vegetable oils (Biodiesel may be prepared from different oils, catalysts and determination of their physical properties viz viscosity, surface tension, flash point .

Spotting

In spotting there should be 5 spots related with instruments and techniques as per syllabus ; time of spotting is 20 minutes

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Semester 4
ELECTIVE PAPERS
Group-C
PRACTICAL PAPER : LC-8-C

CHEMISTRY LAB 8C

Time : 7 Hours

Max. Marks :50 (40 for external 10 for internal)

- A. Experiments of AR, VR, Virtual Laboratory, Molecular models related with simple, complex, polymeric inorganic / organic molecules and methods of analysis (At least two) (10% marks in internal as well as in external)
- B. Designing / Fabrication of low cost instruments or techniques / Green audit of campus, town, city etc. (10% marks in internal as well as in external)
- C. Experiments based on Indian Knowledge system in chemical sciences (10% marks in internal as well as in external)
- D. Spotting – this should include at least five major instruments other than glassware, charts etc. (10% marks in internal as well as in external)
- E. Seminar (10% marks in internal as well as in external)
- F. Project work followed by presentation. The project work should be allotted by a committee constituted at institute level in the beginning of the semester IV and a place / space / workstation should be provided to the students by the institution for the completion of project. The presentation should be in front of a panel and a proper record with geotagged photographs should be maintained. (50% marks in internal as well as in external.)

Semester 4

ELECTIVE PAPERS

Group-D

PRACTICAL PAPER : LC-7-D

CHEMISTRY LAB 7D

Time : 7 Hours

Max. Marks :50 (40 for external 10 for internal)

A Electroanalytical techniques

Polarographic Method:-

- (i) Determination of half wave potential & metal ions eg. Cadmium (II), Mercury (II), Copper (II) etc.
- (ii) Determination of metal-ions, eg. Cadmium (II), Mercury (II), Copper (II) etc, using wave height concentration cell or standard addition.
- (iii) Investigation of the influence of dissolved oxygen.
- (iv) Determination of lead and copper in steel.

Amperometric Method

- (i) Determination of lead with std. potassium dichromate solution
- (ii) Determination Nickel (ii) with dimethyl glyoxime.

- (iii) Determination of Zinc with EDTA
- (iv) Determination of water content of salt hydrate

B. Other advance analytical methods -

- (i) Thermal analysis - Thermal composition of calcium oxalate, copper sulphate, calcium sulphate, hydrate.
- (ii) Electro Gravimetric analysis- Separation & determination of nickel & carbonate.
- (iii) Atomic absorption spectroscopy- Determination of zinc & copper
- (vi) Flame photometry- Determination of Sodium, calcium, magnesium & potassium.
- (v) IR Spectro photometry- Sample preparation, Identification of functional groups.
- (vi) Experiments related with computational and virtual chemistry may be designed and performed.

C. Interdisciplinary Green chemistry experiment (should be performed where more than one special paper is being taught).

Preparation and characterization of Biodiesel from vegetable oils (Biodiesel may be prepared from different oils, catalysts and determination of their physical properties viz viscosity, surface tension, flash point. Analysis of quality of milk by using lactometer.

Spotting

In spotting there should be 5 spots related with instruments and techniques as per syllabus ; time of spotting is 20 minutes

IKS : Applied Chemical Science / Technology in Indian Knowledge system

Semester 4

ELECTIVE PAPERS

Group-D

PRACTICAL PAPER : LC-8-D

CHEMISTRY LAB 8D

Time : 7 Hours

Max. Marks :50 (40 for external 10 for internal)

- A. Experiments of AR, VR, Virtual Laboratory, Molecular models related with simple, complex, polymeric inorganic / organic molecules and methods of analysis (At least two) (10% marks in internal as well as in external)
- B. Designing / Fabrication of low cost instruments or techniques / Green audit of campus, town, city etc. (10% marks in internal as well as in external)
- C. Experiments based on Indian Knowledge system in chemical sciences (10% marks in internal as well as in external)

- D. Spotting – this should include at least five major instruments other than glassware, charts etc. (10% marks in internal as well as in external)
- E. Seminar (10% marks in internal as well as in external)
- F. Project work followed by presentation. The project work should be allotted by a committee constituted at institute level in the beginning of the semester IV and a place / space / workstation should be provided to the students by the institution for the completion of project. The presentation should be in front of a panel and a proper record with geotagged photographs should be maintained. (50% marks in internal as well as in external.)

Books Suggested:

- 1. Inorganic Experiments, J. Derek Woollins, VCH.
- 2. Microscale Inorganic Chemistry, Z. Sqafran, R.M Pike and M.M. Singh, Wiley.
- 3. Practical Inorganic Chemistry, G. Marr and B. W. Rockelt, Van Nostrand.
- 4. The Systematic Identification of Organic Compounds, R.L Shriner and D.Y. Cutin.
- 5. Semimicro Qualitative Organic Analysis, N.D. Cheronis, J.B. Entriinand E.M. Hodnett.
- 6. Experimental Organic Chemistry, M.P. Doyle and W.S. Mungall.
- 7. Small Scale Organic Preparations, P.J. Hill.
- 8. Organometallie Synthesis, J.J. Fisch and R.B. King, Academic.
- 9. Experimental Physical Chemistry, D.P. Shoemaker, C.W. Garland and J.W. Niber, McGrawHill Interscience.
- 10. Findlay's Practical Physical Chemistry, revised B.P. Levitt, Longman.
- 11. Experiments in Physical Chemistry, J.C. Ghosh, Bharti Bhavan.