PREAMBLE

The syllabi of M.Sc programmes in Chemistry offered in the affiliated colleges of the University under Semester system have been revised and the revised syllabi are to be effective from 2013 admission. There are three independent PG programmes in Chemistry, namely M.Sc. Programme in Branch III - Chemistry, M.Sc. Programme in Branch IV - Analytical Chemistry and M.Sc. Programme in Branch V - Applied Chemistry. All these three PG programmes are equivalent in all respect for employment and higher studies. Each of these three PG programmes shall extend over a period of two academic years comprising of four semesters, each of 450 hours in 18 weeks duration. The syllabi and scheme of examinations of these three programmes are detailed below. The theory courses of the first three Semesters and the practical courses of the first two semesters of the three programmes are common, and therefore, the examinations of these three PG programmes are to be conducted with common question papers for the first three semesters by a common Board of Examiners. These syllabi are effective from 2013 admission in affiliated colleges of the university.
# M.Sc. PROGRAMME IN BRANCH III - CHEMISTRY

(Revised syllabus under semester system with effect from 2013 admission)

SYLLABUS AND SCHEME OF EXAMINATION

<table>
<thead>
<tr>
<th>Course No. and Title</th>
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<th>Duration of ESA in hours</th>
<th>Marks for CA</th>
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*Distribution of teaching hours/week: Theory- 15 hours, Practicals- 10 hours (1 hour for Seminar)

| **SEMESTER II***                            |   |   |                          |              |              |             |
| CH 221 Inorganic Chemistry II               | 5 |   | 3                        | 25           | 75           | 100         |
| CH 222 Organic Chemistry II                 | 5 |   | 3                        | 25           | 75           | 100         |
| CH 223 Physical Chemistry II                | 5 |   | 3                        | 25           | 75           | 100         |
| CH 214 Inorganic Practicals I               |   | 3 | 6                        | 25           | 75           | 100         |
| CH 215 Organic Practicals I                 |   | 3 | 6                        | 25           | 75           | 100         |
| CH 216 Physical Practicals I                |   | 4 | 6                        | 25           | 75           | 100         |
| **Total marks for Semester II**             |   |   |                          |              |              | 600         |

*Distribution of teaching hours/week: Theory- 15 hours, Practicals- 10 hours (1 hour for Seminar)
### SEMESTER III*

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<tr>
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Total marks for semester III: 300

*Distribution of teaching hours/week: Theory - 15 hours, Practicals - 10 hours (1 hour for Seminar)

### SEMESTER IV*

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Total marks for Semester IV: 600
Grand total (for semesters I-IV): 1800

*Distribution of teaching hours/week: Theory - 15 hours, 10 hours for discussion on project (1 hour for Seminar)

**Each student has to choose either (a), (b), (c) as elective in accordance with the Dissertation chosen.
M.Sc. PROGRAMME IN BRANCH III - CHEMISTRY

(Revised syllabus under Semester System w.e.f. 2013 Admission)

SEMESTER I

CH 211 INORGANIC CHEMISTRY - I

Total 90 h

Unit I  Noble gases, halogens, isopoly and heteropoly acids  18 h

  Noble gas compounds: Preparation, properties, structure and bonding. Halogens in positive oxidation states. Preparation, properties, structure, bonding and uses of inter halogen compounds, pseudo halogens, poly halide ions. Astatine: Synthesis, stability and properties.

  Preparation, properties and structure of isopoly and heteropoly acids of Mo and W. Classification, preparation, properties and structure of borides, carbides, nitrides and silicides. Classification and structure of silicates. Properties and structure of aluminosilicates and zeolites. Preparation, properties and applications of silicones.

Unit II  Coordination chemistry-I: Theories of metal complexes  18 h


Unit III Analytical principles 18 h


Unit IV Nanomaterials 18 h

General introduction to nanomaterials and emergence of nanotechnology, Moore’s law, synthesis and properties of fullerenes and carbon nanotubes, synthesis of nanoparticles of gold, silver, rhodium, palladium and platinum. Techniques of synthesis- electroplating and electrophoretic deposition, conversion through chemical reactions and lithography. Thin films- chemical vapour deposition and atomic layer deposition techniques.

Elementary idea of characterization of nanomaterials using XRD powder, TEM, AFM, SEM and STM techniques.


Unit V Chemistry of natural environmental processes 18 h.


References

15. C.P. Poole Jr. and J. Owens,’ Introduction to Nanotechnology,’ Wiley India.

**CH 212 ORGANIC CHEMISTRY - I**

Total 90 h

**Unit I Stereochemistry of organic compounds 18 h**

Nomenclature of organic compounds, Fused polycyclic hydrocarbons, Bridged polycyclic hydrocarbons, Bridged fused systems, Spiroyclic hydrocarbon systems, Heterocyclic systems, Metal organic compounds.


**Unit II Structure, reactivity and intermediates 18 h**

Unit III. Substitution and elimination reactions

Nucleophilic substitution at sp\(^3\) carbon, its mechanisms and stereochemical aspects. Effect of solvent, leaving group and substrate structure. \(S\text{N}^1\), \(S\text{N}^2\), \(S\text{N}1^1\), \(S\text{N}2^1\), \(S\text{Ni}\) reactions. Neighbouring group participation. Non-classical carbocations. Elimination reactions leading to C=C bond formation and their mechanisms. E1, E2 and E1CB mechanisms. Stereoaspects of C=C bond formation. Effect of leaving group and substrate structure. Hoffmann and Saytzeff elimination. Cis elimination. Competition between \(S\text{N}^1\) and \(S\text{N}^2\), E1 and E2, Alkyl halides as survival compounds

Unit IV Reactivity of unsaturated systems


Unit V Separation techniques


References


**CH 213-PHYSICAL CHEMISTRY -I**

**Total 90 h**

**Unit I Quantum mechanics**


Application to simple systems: Solution of Schrodinger wave equation for a free particle, particle on a ring, particle in 1D box, particle in 3D box, separation of variables, degeneracy.

One dimensional Harmonic oscillator- Complete solution. Hermite polynomials, recursion formula, features of the wave functions.


**Unit II Molecular symmetry** 18 h


Reduction formula, reduction of reducible representation to IRs. Transformation properties of atomic orbitals. Hybridisation: identification of atomic orbitals taking part in hybridisation of triangular planar, square planar, triagonal bipyramidal, square pyramidal and tetrahedral molecules. Molecular symmetry and optical activity.
Unit III Basics of chemical thermodynamics


Unit IV Chemical kinetics

Complex reactions, Reversible, Consecutive, Concurrent and branching reactions. Free radical and chain reactions. Steady state treatment. Reactions like H\textsubscript{2}-Cl\textsubscript{2}, H\textsubscript{2}-Br\textsubscript{2}, and decompositions of ethane, acetaldehyde and N\textsubscript{2}O\textsubscript{5}. Rice-Herzfeld mechanism, Potential energy surfaces-adiabatic and non adiabatic curve crossing processes. Unimolecular reaction. Lindemann treatment. Semenoff-Hinshelwood mechanism of chain reactions and explosion.


Theories of Reaction rate: Arrhenius equation and its limitations, activation energy, Collision theory and absolute reaction rate theory. Free energy of activation and volume of activation. Thermodynamic formulation of reaction rate. Effects of pressure and volume on the velocity of gas reaction.


**Unit V  Gases, liquids and liquid crystals**

18 h


Liquid crystals: Mesomorphic state, types, examples and applications of liquid crystals. Theory of liquid crystals.

**References**

1 I.N. Levin, “Quantum Chemistry”, Prentice Hall


5 T. Angel, “Quantum Chemistry and Spectroscopy”, Pearson Education.

6 P. W. Atkins, R. S. Friedman, ”Molecular Quantum Mechanics”, Oxford University Press.

8 F.A.Cotton,” Chemical Applications of Group Theory”, Wiley Eastern


14 S.Glastone, “Thermodynamics for Chemists”,


CH 214 INORGANIC CHEMISTRY PRACTICALS -1
Total 125 h

1. Separation and identification of rare/less familiar cations such as Ti, W, Mo, Th, Zr, V, U and Li

2. Volumetric estimation using EDTA, ammonium vanadate, ceric sulphate etc.

3. Colorimetric/spectrophotometric estimation of Cr, Fe, Mn, Ni, Cu etc.

4. Preparation of metal complexes: selection can be made from the following or any other from the existing literature.
   i) [Co(NH$_3$)$_6$]Cl$_3$, (ii) [Cu(NH$_3$)$_4$]SO$_4$ (iii) K$_3$[Cr(C$_2$O$_4$)$_3$]
   iv). K$_3$[Fe(C$_2$O$_4$)$_3$], v). Cis and trans isomers of [Co(en)$_2$Cl$_2$]Cl

iv). [Cr(en)$_3$]Cl$_3$

References


CH 215 ORGANIC PRACTICALS -1
Total 125 h

A. Separation and identification of organic compounds

1. Quantitative wet chemistry separation of a mixture of two components by solvent extraction
2. Purification of the separated samples by boiling and crystallization.

3. TLC of the purified samples along with the mixture in same TLC plates (if not possible use separate plates) and calculation of Rf values.

**B. Separation of a mixture of by column chromatography**

1) Malachite green and methylene blue 2) O-nitroaniline and p-nitroaniline.

**C. Preparation of compounds by two stages.**

TLC analysis of the products and original compound in the same plate and measurement of Rf values. Recording UV, IR, NMR and mass spectrum of synthesized compounds.

1) Acetanilide- \( \rightarrow \) p-nitroacetanilide \( \rightarrow \) p-nitroaniline

2) Methylbenzoate \( \rightarrow \) m-nitromethylbenzoate \( \rightarrow \) m-nitrobenzoic acid

3) Acetanilide- \( \rightarrow \) p-bromoacetanilide \( \rightarrow \) p-bromooaniline

**E. Green Organic Chemistry experiments**

1) Acetanilide- \( \rightarrow \) p-bromoacetanilide (KBr and CAN)

2) Benzophenone \( \rightarrow \) Benzpinacol (photoreduction)

**References**

3. Vishnoi, Practical Organic Chemistry, Vikas
5. F G Mann and BC saunders, Practical Organic Chemistry, Pearson
7. C.E Bella and DF Taber, Organic Chemistry Laboratory, Thomson
8. Nelson Practical Biochemistry, Wiley
11. Monograph on green laboratory experiments, DST , Govt of India.
12. [http://sdbs.riodb.aist.go.jp/sdbs/cgi-bin/direct_frame_top.cgi](http://sdbs.riodb.aist.go.jp/sdbs/cgi-bin/direct_frame_top.cgi)
CH 216 PHYSICAL PRACTICALS –I

Total 125 h

1. Adsorption

Freundlich and Langmuir isotherms for adsorption of acetic/oxalic acid on active charcoal.

Determination of concentration of acetic/oxalic acid.

2. Kinetics

Determination of rate constant of acid hydrolysis of methyl acetate.

Determination of Arrhenius parameters.

Determination of concentration of given acid.

Determination of rate constant of the saponification of ethyl acetate and evaluation of Arrhenius parameters.

Determination of rate constant of reaction between $K_2S_2O_8$ and KI.

Study the kinetics of iodination of acetone in acid medium.

3. Phase rule

**Solid-liquid equilibria** – Construction of phase diagram and determination of the composition of unknown mixture (naphthalene/biphenyl, naphthalene/benzophenone, naphthalene/diphenyl amine)

Construction of phase diagram with congruent melting point- naphthalene/meta-dinitrobenzene

**Partially miscible liquid pairs**- CST of phenol-water system.

Effect of impurities (KCl/NaCl/succinic acid) on the miscibility temperature of phenol-water system and hence the concentration of given unknown solution.

Three component system- Construction of ternary phase diagram of acetic acid-chloroform-water system and hence the composition of given homogeneous mixture.
Construction of tie-line.

4. Distribution law

Distribution coefficient of iodine between CCl₄ and water

Distribution coefficient of benzoic acid between toluene and water.

Determination of the equilibrium constant of the reaction KI+I₂ → [KI₃] and hence the concentration of given KI.

Distribution coefficient of ammonia between chloroform and water.

Determination of equilibrium constant of copper-ammonia complex by partition method or coordination number of Cu²⁺ in copper-ammonia complex.

Determination of hydrolysis constant of anilinium hydrochloride.

5. Dilute solutions

Determination of K_f of solid solvent, molar mass of non-volatile solute, mass of solvent and composition of given solution (Solvent- Naphthalene/Biphenyl/ Benzophenone etc. Solute- Naphthalene/ Biphenyl/ Diphenylanmine etc)

Determination of vant Hoff’s factor for benzoic acid in Naphthalene.

Determination of atomicity of sulphur.

6. Transition temperature

Determination of K_f of salt hydrate, molar mass of solute, mass of salt hydrate and composition of given solution (Solvent- Na₂S₂O₃.5H₂O/CH₃COONa.3H₂O, Solute- glucose, sucrose, urea)

7. Thermochemistry

Determination of the concentration of given strong acid/alkali.

Thermometric titration of NaOH Vs standard HCl.

Heat of displacement of Cu²⁺ by Zn.
Determinant of the heat of ionisation of acetic acid.

References


4) A. M. James, and F. E. Pichard, “Practical Physical Chemistry”, Longman.


6) B. Viswanathan, “Practical Physical Chemistry”, Viva Publications.


SEMESTER II

CH 221 INORGANIC CHEMISTRY –II

Total 90 h

Unit I  Sulphur, nitrogen, phosphorus and boron compounds  18 h

Sulphur-nitrogen compounds: Tetrasulphur tetranitride, disulphur dinitride and polythiazyl $S_nN_y$ compounds. S-N cations and anions. Other S-N compounds. Sulphur-phosphorous compounds:

Molecular sulphides such as $P_3S_3$, $P_6S_7$, $P_8S_9$ and $P_4S_{10}$. Phosphorous-nitrogen compounds: Phosphazines. Cylco and linear phosphazines. Other P-N compounds

Unit II Coordination chemistry-II: Spectral and magnetic properties of transition metal complexes 18 h

Electronic spectra of metal complexes- Term symbols of $d^n$ system, Racah parameters, splitting of terms in octahedral and tetrahedral fields. Correlation diagrams for $d^n$ and $d^{10-n}$ ions in octahedral and tetrahedral fields (qualitative approach), $d-d$ transition, selection rules for electronic transition-effect of spin orbit coupling and vibronic coupling

Interpretation of electronic spectra of complexes- Orgel diagrams, Tanabe-Sugano diagrams, Calculation of $Dq$, $B$ and $\beta$ (Nephelauxetic ratio) values, charge transfer spectra.


Unit III Crystalline state 18 h


**Unit IV Lanthanides and actinides**


**Unit V Solid state chemistry**


Intrinsic and extrinsic semiconductors, doping of semiconductors and conduction mechanism, the band gap, temperature dependence of conductivity, carrier density and carrier mobility in semiconductors, synthesis and purification of semiconducting materials, single crystal growth, zone refining, fractional crystallization, semiconductor devices, rectifier transistors, optical devices, photoconductors, photovoltaic cells, solar batteries.

**References**

5. J. C. Bailar, ‘Chemistry of Coordination Compounds’, Reinhold.

CH 222 ORGANIC CHEMISTRY- 11

Unit I Molecular rearrangement and transformation reactions 18 h

Unit II Aromaticity and symmetry controlled reactions 18 h


Unit III Organic photochemistry 18 h


Unit IV Chemistry of natural products and biomolecules 18 h

Introduction to primary and secondary metabolites in plants. Extraction methods of chemical constituents from plants, such as fractionation using solvents, specific extraction of alkaloids and supercritical fluid extraction. Characterizations of isolated compounds (terpenes, sterols, alkaloids, carbohydrates, flavonoids and poly phenols) by colour reactions and spray reagents. Biosynthesis of terpenes from mevalonic acid and sterols from squalene. Structure elucidation of ocimene monoterpene, classification of pigments, structure elucidation of β –carotene. Structural differences between a triterpene and a sterol. Synthesis of quercetin, synthesis of testosterone, androsterone, estrone and progesterone. Determination of carbon skeleton of alkaloids (Hofmann, Emde and Von Braun degradation methods). Structural elucidation of ephedrine, nicotine , atropine,hygrine.

Unit V Physical organic chemistry 18 h


References

1. L.M. Harwood, Polar rearrangements, Oxford University.
5. P.Y. Bruice, Organic chemistry, Prentice Hall.
12. R.J. Simmonds, Chemistry of Biomolecules, Royal Society of Chemistry.
13. J. Mann and others, Natural products- Their Chemistry and Biological Significance, Longmann
16. N.R. Krishnaswamy, Chemistry of Natural Products, A Unified Approach.
17. N. R. Krishnaswamy, Chemistry of Natural Products, A Laboratory Hand Book.
19. J.B. Harborne, Phytochemical Methods, Chapman and Hall.
Unit I  Chemical Bonding

Approximate methods: Variation method- Variation theorem and its proof. Linear variation functions. Secular equations and secular determinants.

Perturbation method- Successive correction to an unperturbed problem. Detailed treatment of first order non-degenerate case only. LCAO-MO Theory- MO theory of $H_2^+$ and $H_2$. MO treatment of other homo diatomic molecules Li$_2$, Be$_2$, B$_2$, C$_2$, N$_2$, O$_2$ and F$_2$. MO treatment of hetero diatomic molecules LiH, CO, NO and HF. Spectroscopic term symbols for homo diatomic molecules.

Valance bond theory of H$_2$. Quantum mechanical treatment of SP, SP$^2$ and SP$^3$ Hybridisation.

HMO theory of conjugated π-systems. Bond order and charge density calculations. Free valance. Application of HMO method to ethylene, allyl system, butadiene and benzene.

Secondary bond forces: ion dipole, dipole-dipole, ion-induced dipole, London dispersion forces.

Unit II  Spectroscopy –I

Microwave spectroscopy: Rotational spectrum, Intensity of spectral lines, calculation of inter nuclear distance. Non-rigid rotors and centrifugal distortion. Rotational spectra of polyatomic molecules-linear and symmetric top molecules. Introduction to instrumentation.


Vibrational spectra of polyatomic molecules: Normal modes, classification of vibrational modes into stretching (asymmetric, symmetric), bending, parallel and perpendicular vibrations. Finger print region and group frequencies. Introduction to FTIR and instrumentation.


Unit III  Applications of thermodynamics 18 h

Phase equilibria: Criteria of Equilibrium. Derivation of phase rule Discussion of two component systems forming solid solutions with and without maximum or minimum in freezing point curve. Systems with partially miscible solid phases.


Unit IV  Statistical mechanics –I 18 h


The Partition functions. Partition function for free linear motion, for free motion in a shared space, for linear harmonic vibration.

**Unit V Electrochemistry**


Fuel cells- H₂-O₂ fuel cell, fuel cell for high temperature applications.


**References**

1. I.N. Levine, "Quantum Chemistry", Printice Hall.


J.Rajaram, J.C.Kuriakose, ”Thermodynamics”, S Chand and Co.

I.Pregogine,”Introduction to Thermodynamics of Irreversible Process”, Inter Science.

M.C.Gupta,”Elements of Statistical thermodynamics”, New Age International.


C.Kalidas, M.V. Sangaranarayanan,”Non-equilibrium Thermodynamics”, Macmillian India.

McQuarrie, “Statistical Mechanics”, Orient Longman.


S.Glasstone, “Introduction to Electrochemistry”,


SEMESTER III

CH 231 INORGANIC CHEMISTRY - III

Total 90 h

Unit I Organometallic compounds 18 h


Unit II Coordination chemistry-III: Reactions of metal complexes 18 h

Energy profile of a reaction - Thermodynamic and kinetic stability, Classification of ligand substitution reactions - kinetics and mechanism of ligand substitution reactions in square planar complexes, trans effect- theory and synthetic applications.

Kinetics and mechanism of octahedral substitution- water exchange, dissociative and associative mechanisms, base hydrolysis, racemization reactions, solvolytic reactions (acidic and basic)

Electron transfer reactions: Outer sphere mechanism- Marcus theory, inner sphere mechanism- Taube mechanism. Photochemical reactions- substitution and redox reactions of Cr(III), Ru(II), and Ru(III) complexes. Photo-isomerisation and photo-aquation reactions of metal complexes.

Unit III Bioinorganic chemistry 18 h

Essential and trace elements in biological systems, structure and functions of biological membranes, mechanism of ion transport across membranes, sodium-potassium pump. Photosynthesis, porphyrin ring system, chlorophyll, PS I and PS II. Synthetic model for photosynthesis. Role of calcium in biological systems.

**Unit IV Electrical and magnetic properties of solids** 18 h


**Unit V Nuclear chemistry** 18 h


**References**

5. V. Raghavan, ‘Materials Science and Engineering’, a first course, Prentice Hall

CH 232 ORGANIC CHEMISTRY-111

Total 90 h

Unit 1 UV-VIS, IR and Mass spectroscopy 18 h

instrumentation. Organic mass spectroscopy. EI, CI, FAB, Electrospray and MALDI ion sources. Magnetic, High resolution (Double focusing), TOF and quadruple mass analysers. Characteristic EIMS fragmentation modes and MS rearrangements. Mass spectral fragmentation patterns of long chain alkanes, alkenes, alkynes, carbonyl, nitro, amino and carboxy compounds. Strategies for the analysis of mass spectra.

**Unit II  NMR Spectroscopy and structure elucidation**  18 h

Theory of NMR spectroscopy, chemical shifts, anisotropic effects and coupling constant. Spin-spin interactions in typical systems. First order and second order spectra. Simplification methods of complex spectra by high field NMR, shift reagents, chemical exchange and double resonance. Theories of FT NMR (1D NMR), 2D NMR and $^{13}$C NMR spectroscopies. $^{13}$C NMR chemical shifts. Instrumentation of NMR. Applications of NOE, APT, DEPT, INEPT and 2-DNMR and INADEQUATE, HOHA spectroscopies. Introduction to 3D NMR. Spectral interpretations and structure identification. Spectral interpretation using actual spectra taken from standard texts. Solving of structural problems on the basis of numerical and spectrum based data.

**Unit III Molecular recognition and supramolecular chemistry**  18 h


**Unit IV Medicinal chemistry**  18 h

Retrosynthetic analysis and disconnection approach. Synthetic strategy and synthons,
Combinatorial organic synthesis, introduction, methodology, automation, solid supported and solution phase synthesis, study of targeted or focused libraries and small molecule libraries, Application—drug discovery.


Unit V Green chemistry


References

5. H.O. House, Modern synthetic reactions, Benjamin Cummins.
9. R.M. Merhotra and Singh, Organometallic chemistry.


11. J.M. Lehn, Supramolecular chemistry, VCH.


13. V.K. Ahluwalia and Mahu Chopra, Medicinal chemistry.


15. Ashutosh Kar, Medicinal chemistry.


17. P.Y. Bruice, Organic chemistry, Prentice Hall.

18. P.T. Anastas, and J.C. Warner, Green chemistry, Theory and Practice, OUP.


**CH 233 Physical Chemistry -III**

**Total 90 h**

**Unit I Computational chemistry.**

18 h

Introduction to computational chemistry, concept of potential energy surface (PES), stationary point, saddle point and geometry optimisation.

Basis sets, STO, Gaussian functions and its properties, GTO, contracted Gaussians, minimal, split valence, polarised and diffused basis sets.

Introduction to SCF. Wave function for open shell state, RHF, ROHF and URHF. Model Chemistry. Brief description of computational methods- ab-initio, semiempirical and density
functional and molecular mechanics methods. Construction of Z-matrix for simple molecules- H₂O, H₂O₂, H₂CO, CH₃CHO, NH₃, and CO₂.

**Unit II Spectroscopy II**

18 h


ESR spectroscopy: Electron spin. Interaction with magnetic field. Kramer’s rule. The g factor. Determination of g values. Fine structure and hyperfine structure. Elementary idea of ENDOR and ELDOR.


Photoelectron spectroscopy. Introduction to UV photoelectron and X-ray photoelectron spectroscopy.

**Unit III Statistical mechanics II**

18 h


Unit IV Surface chemistry and catalysis 18 h


Surface films: different types, Surface pressure and Surface potential, and their measurements and interpretation.


Catalysis: Mechanism and theories of homogeneous and heterogeneous catalysis. Enzyme catalysis, Bimolecular surface reactions. Langmuir – Hinshelwood mechanism

Instrumental methods of catalyst characterization- diffraction and thermal methods, spectroscopic and microscopic techniques.

Unit V Electro Analytical and spectrophotometric methods. 18 h

Flame emission and atomic absorption spectrometry. Instrumentation for AAS. The flame characteristics. Atomiser used in spectroscopy. Hollow cathode lamp. Interference in AAS. Application of AAS.

References

10. A. W. Adamson,”Physical Chemistry of Surfaces”, Wiley India.
12. G. A. Somorjai, Y. Li, Introduction to Surface Chemistry and Catalysis.
15. McQuarrie, “Statistical Mechanics”, Orient Longman

18 D. Chandler. Introduction to Modern Statistical Mechanics, Oxford University Press.


**CH 234 Inorganic Chemistry Practicals -II** Total-125 h

1. Estimation of simple mixture of ions (involving quantitative separation) by volumetric and Gravimetric methods.

2. Analysis of typical alloys and ores

3. Ion exchange separation of binary mixtures.

4. Spectral Interpretation of metal complexes using IR, UV-Vis. spectral data. Supplementary information like metal estimation, CHN analysis, conductivity measurements and magnetic measurements to be provided to the students. Assessment is based on arriving at the structure of the complex and assignment of IR spectral bands.

5. Interpretation of TG and DTA curves of metal oxalates/acetates/sulphates/chlorides in hydrated forms. Assessment is based on the identification of various stages.

**References**


4. Willard, Merrit and Dean, ‘Instrumental Methods of Analysis,’


CH 235 ORGANIC PRACTICALS-II

Total 125 h

A. Volumetric estimation of
1) Aniline  2) Phenol  3) glucose
4) Iodine value and saponification value of coconut oil


C. Spectral identification ( UV, IR, $^1$H NMR, $^{13}$C NMR, EI mass) of Organic compounds from a library of organic compounds

D. Separations of mixtures by Paper Chromatography
1) Separation of amino acids    2) Separation of dyes

E) Three stage preparation
1) Benzaldehyde $\rightarrow$ Benzoin (green synthesis with thiamine HCl) $\rightarrow$ benzil
   $\rightarrow$ benzilic acid
2) Phthalic acid $\rightarrow$ Phthalic anhydride $\rightarrow$ pthalimide $\rightarrow$ anthranilic acid

References
3. Vishnoi, Practical Organic Chemistry, Vikas
4. R.M Silverstein, Spectrometric identification of Organic compounds
5. F G Mann and BC saunders, Practical Organic Chemistry, Pearson
7. C.E Bella and DF Taber, Organic Chemistry laboratory, Thomson
8. Nelson Practical Biochemistry, wiley
10. P.D.L Lampman and Chriz, Introduction to organic Laboratory techniques, College publishing,
11. Monograph on green laboratory experiments, DST, Govt of India.
12. http://s dbs.riodb.aist.go.jp/s dbs/cgi-bin/direct_frame_top.cgi

**CH 236 PHYSICAL PRACTICALS –II**

1. **Conductometry**

Determination of strength of strong and weak acids in a mixture
Determination of strength of a weak acid.
Determination of solubility product of a sparingly soluble salt (PbSO₄, BaSO₄ etc.)
Hydrolysis of NH₄Cl or CH₃COONa or aniline hydrochloride
Determination of order of reaction, rate constant and energy of activation for saponification of ethyl acetate
Precipitation titrations.
Determination of critical micellar concentration (CMC) of sodium lauryl sulphate from measurement of conductivities at different concentrations.
Equivalent conductance at infinite dilutions and verification of Kohlraush’s Law.
Determination of Onsager constants.

2. **Potentiometry**

Determination of emf of Daniel cell.
Determination of the emf of various ZnSO₄ solutions and hence the concentration of unknown ZnSO₄ solution.
Determination of valency of mercurous ion.
Determination of temperature dependence of EMF of a cell
Determination of stoichiometry and formation constant of silver-ammonia complex.
Determination of activity and activity constant of electrolytes.
Determination of thermodynamic constants of reactions.
pH metric titrations.
Acid alkali titrations using Quinhydrone electrode.
Titrations(double) involving redox reactions – Fe$^{2+}$ Vs KMnO$_4$, K$_2$Cr$_2$O$_7$, Ce(NH$_3$)$_3$SO$_4$ and KI Vs KMnO$_4$
Determination of strengths of halides in a mixture.
Determination of pH of buffer solutions and hence to calculate the $E_0$ of quinhydrone electrode

3. **Spectrophotometry**
Verification of Beer-Lambert’s law.
Absorption spectra of conjugated dyes.
Determination of concentration of potassium dichromate and potassium permanganate in a mixture.
To study the complex formation between Fe$^{3+}$ and salicylic acid.
Determination of pKa of an indicator.

4. **Polarimetry**
Measurement specific rotation of glucose.
Determination of specific rotation of sucrose
Determination of unknown concentration of glucose solution.
and rate constant of its hydrolysis in presence of HCl

5. **Polarography** :
Determination of half wave potential $E \frac{1}{2}$ and unknown concentration of Cd$^{2+}$ ion.
Determination of concentrations of metal ions in a mixture.

6. **Surface tension**
Determination of surface tension of various liquids by Stalagmometric method (drop number / drop weight)
Determination of parchors of molecules and various groups.
Determination of concentration of a mixture.
Determination of surface tension and paracho of liquids using double capillary method.

7. **Refractometry**
Determination of molar refraction of pure liquids
Determination of concentration of KCl solution/glycerol solution
Determination of solubility of KCl in water.
Determination of molar refraction of solid KCl

Study the stoichiometry of potassium iodide-mercuric iodide complex.

Determination of concentration of KI solution.

8. **Viscosity**

Determination of viscosity of various liquids using Ostwald’s viscometer.

Determination of unknown composition of given liquid mixture like toluene-nitrobenzene.

Verification of Kendall’s relation.

Verification of Jon Dole’s equation.

**References**


A. M. James, and F. E. Pichard, “Practical Physical Chemistry”, Longman.


B. Viswanathan, “Practical Physical Chemistry”, Viva Publications.


**SEMESTER IV**

**CH 241 (a) ADVANCED INORGANIC CHEMISTRY**

Total 90 h

**Unit 1 Spectroscopic methods in inorganic chemistry-I**  18 h

Infrared and Raman spectroscopy: Vibrational modes, group frequencies of infrared systems, factors affecting the group frequencies, study of hydrogen bonding effects, infrared spectra of coordination compounds. Structural elucidation of coordination compounds.
containing the following molecules/ions as ligands - NH$_3$, H$_2$O, CO, NO, OH$^-$, SO$_4^{2-}$, CN$^-$, SCN$^-$, NO$_3^-$, NO$_2^-$, CH$_3$COO$^-$ and X$^-$ (X= halogen).

Changes in ligand vibration on coordination with metal ions. Vibrational spectra of metal carbonyls- CD and ORD spectra of metal complexes.

Physical characterization of inorganic compounds by UV, NQR and MS techniques.

**Unit II Applications of group theory**

Hybrid orbitals and molecular orbitals for simple molecules. Transformation properties of atomic orbitals. Hybridization schemes for σ and π bonding with examples. MO theory for AB$_n$ type molecules. Molecular orbitals for regular octahedral, tetrahedral and metal sandwich compounds.


Symmetry and selection rules: Symmetry properties of common orbitals. Application of character tables to infrared and Raman spectroscopy. Infrared and Raman active modes for C$_{2v}$, C$_{3v}$ and D$_{4h}$

**Unit III Spectroscopic methods in Inorganic chemistry -II**

ESR spectra of metal complexes: Hyperfine splitting and A parameter, g values, zero field splitting and Kramers degeneracy. Application to Cu(II) complexes and inorganic free radicals such as PH$_4^-$, F$_2^-$ and [BH$_3$]$^-$.

Nuclear Magnetic Resonance Spectroscopy: The contact and pseudocontact shifts, factors affecting nuclear relaxation, some applications including biological systems, an overview of NMR of metal nuclides with emphasis on $^{31}$P and $^{19}$F NMR.

Mossbauer Spectroscopy: Basic Principles, spectral parameters and spectrum display. Application of the technique to the studies of iron and tin complexes.
Unit IV  Metal-metal bonds and metal clusters  18 h


Unit V  Bioinorganic chemistry  18 h


References

7. V. Raghavan, Materials Science and Engineering, a first course, Prentice Hall.
Unit I Reagents in organic synthesis


Unit II Organometallic chemistry

Preparation of organo Mg, Al, Li, Cu, Zn, Cr, Fe, Ce and sulphur stabilised compounds. Reactions of Grignard reagents in organic synthesis. Alkylation, oxirane addition, carbon dioxide addition, carbonyl addition, enone addition (1,2 and 1,4additions), reduction, conjugate addition and enolisation reactions. Selectivity in Grignard reactions. Reactions of organo Li reagents, Li exchange reaction, its use in the preparation of RLi compounds,

**Unit III Organic synthesis**

18 h


**Unit IV Methods in organic synthesis**

18 h


**Unit V Chemistry of biopolymers and polymers**

18 h


**References**


2. W. Kemp, Organic spectroscopy, Longman


5. M.B. Smith, Organic synthesis, Mc-Grow Hill.


7. R.J. Simmonds, Chemistry of biomolecules, Royal society of chemistry.

8. Jie Jack Li, Namereactions, Springer


12. Mc Murray, Organic synthesis

13. R.J. Young, Introduction to polymer science, John Wiley and Sons.


17. K.J. Saunders, Organic polymer chemistry, Chapman and Hall.


**SEMESTER IV**

**CH 241(c) ADVANCED PHYSICAL CHEMISTRY**

Total 90 h

**Unit I Applications of group theory**

18 h

Spectroscopic applications: Transition moment integral transition moment operator. Vanishing matrix element. Symmetry selection rule for IR, Raman and electronic spectra. Dipole and polarizability transition moment operator. Identification of IR and Raman active normal modes in molecules coming under various point groups such as \(C_{2v}, C_{3v}, C_{4v}, D_{3h}, T_d\) and \(O_h\). Mutual exclusion and complementarity principle of IR and Raman spectra and their use in the identification of molecular structures. Probability of overtone and combination bands. Identification of allowed and forbidden electronic transitions in carbonyl groups. Vibronic transitions.

Application to MO theory: Symmetry adapted LCAO-MO theory of \(\pi\)-bonded hydrocarbons. Projection operator and its use in the construction of wave functions of \(\pi\)-molecular orbitals, secular equations and use of symmetry for simplifying the calculations of energy and wave functions of ethylene, butadiene and carbocyclic systems such as benzene and naphthalene.

**Unit II Exactly solvable systems.**

18 h

Simple Harmonic Oscillator: Wave equation for 1D harmonic oscillator. Complete solution and their properties. Three dimensional Harmonic oscillator. Potential energy in
three dimension and Schrodinger wave equation in Cartesian coordinate. Separation of variables and solution of the equation for energy and wave function. Degeneracy.


Angular momentum, angular momentum operators($L_x,L_y,L_z$ and $L^2$) and their commutation properties. Spherical harmonics as eigen functions of angular momentum operator $L_z$ and $L^2$. Ladder operator method for angular momentum. Space quantisation.

**Unit III Approximate method I**  
18 h

Schrodinger wave equation for He atom and anharmonic oscillator and difficulty to get the exact solution. The Variation method: Variation theorem and its proof. The variation integral and its properties. Variational parameters. Trial wave functions, Illustration of trial wave functions for calculation of H atom and particle in a 1D box as examples.

Trial functions as linear combination of orthonormal functions, linear combinations of functions containing variational parameters as trial functions. Setting up of secular determinants. Variation methods of normal state of He. The SCF method, SCF and variation method. Strength and limitation of the method.

**Unit IV Approximate method II**  
18 h

Time dependant wave equation: Variation in the state of a system with time. Emission and absorption of radiation. The Einstein’s transition probability and its calculation. Selection rules and intensity of spectrum for harmonic oscillator, rigid rotor and hydrogen atom.

Unit V Computational methods


Basis sets: minimal basis set, split valance basis set, polarised basis set and diffused basis set. Model chemistry and notations.

Geometry input- in terms of Cartesian coordinates and internal coordinates. Z-matrix, construction of z-matrices of simple molecules H₂, H₂O, H₂O₂, H₂CO,CH₃CHO, CH₄, C₂H₆ and with dummy atom, CO₂, NH₃,C₆H₆.


Ab-initio method: Hartree-Fock Self Consistent Field method. Slater determinant. Post Hartree-Fock methods- Configuration Interaction(CI) and Moller Plesset(MP)methods.


Comparative study of Molecular Mechanics, Ab-initio method, Semi-empirical method and DFT method of computations.
Each of the students has to carry out original research in a topic in accordance with the Elective paper chosen for Semester IV under the guidance and supervision of a teacher in the concerned Department of the College.

References

5. P. W. Atkins, R. S. Friedman, ”Molecular Quantum Mechanics”, Oxford University Press.

CH 242 DISSERTATION

Each of the students has to carry out original research in a topic in accordance with the Elective paper chosen for Semester IV under the guidance and supervision of a teacher in the concerned Department of the College.
Instructions to Question Papers Setters

The Syllabus of each theory has five units. While setting the question papers, equal weight is to be given to each of the Units for choosing the questions. Each question paper is of 3 hours duration and has three Sections, namely Section A, Section B and Section C constituting a total 75 marks as detailed.

**Section A**- Five questions, one from each Unit containing three short answer questions marked (a), (b), and (c), each of which has 2 marks. One has to answer any two of (a), (b) or (c) from each of the five questions. (2x10 = 20 marks)

**Section B**- Five questions, one from each Unit containing two short essay questions marked (a) and (b), each of which has 5 marks. One has to answer either (a) or (b) from each of the five questions. (5x5 = 25 marks)

**Section C**- Five essay questions, one from each unit having 10 marks. One has to answer any three questions from the five questions asked.(10x3 = 30 marks)
# M.Sc. PROGRAMME IN BRANCH IV - ANALYTICAL CHEMISTRY

(Revised syllabus under semester system with effect from 2013 admission)

## SYLLABUS AND SCHEME OF EXAMINATION

<table>
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*Distribution of teaching hours/week: Theory- 15 hours, Practicals- 10 hours (1 hour for Seminar)

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M.Sc. PROGRAMME IN BRANCH IV – ANALYTICAL CHEMISTRY

(Revised syllabus under Semester System w.e.f. 2013 Admission)

SEMESTER I

CL 211 INORGANIC CHEMISTRY - I

Total 90 h

Unit I Noble gases, halogens, isopoly and heteropoly acids 18 h

Noble gas compounds: Preparation, properties, structure and bonding. Halogens in positive oxidation states. Preparation, properties, structure, bonding and uses of inter halogen compounds, pseudo halogens, poly halide ions. Astatine: Synthesis, stability and properties.

Preparation, properties and structure of isopoly and heteropoly acids of Mo and W. Classification, preparation, properties and structure of borides, carbides, nitrides and silicides. Classification and structure of silicates. Properties and structure of aluminosilicates and zeolites. Preparation, properties and applications of silicones.

Unit II Coordination chemistry-I: Theories of metal complexes 18 h


Unit III Analytical principles 18 h


Unit IV Nanomaterials 18 h

General introduction to nanomaterials and emergence of nanotechnology, Moore’s law, synthesis and properties of fullerenes and carbon nanotubes, synthesis of nanoparticles of gold, silver, rhodium, palladium and platinum. Techniques of synthesis-electroplating and electrophoretic deposition, conversion through chemical reactions and lithography. Thin films- chemical vapour deposition and atomic layer deposition techniques.

Elementary idea of characterization of nanomaterials using XRD powder, TEM, AFM, SEM and STM techniques.


Unit V Chemistry of natural environmental processes 18 h.


References

15. C.P. Poole Jr. and J. Owens, ‘Introduction to Nanotechnology,’ Wiley India.
17. H.V. Jadhav, Elements of Environmental Chemistry.

CL 212 ORGANIC CHEMISTRY - I

Total 90 h

Unit I Stereochemistry of organic compounds 18 h

Nomenclature of organic compounds, Fused polycyclic hydrocarbons, Bridged polycyclic hydrocarbons, Bridged fused systems, Spirocyclic hydrocarbon systems, Heterocyclic systems, Metal organic compounds.


Unit II Structure, reactivity and intermediates 18 h


Unit III. Substitution and elimination reactions 18 h

Nucleophilic susbstitution at sp^3 carbon, its mechanisms and stereochemical aspects. Effect of solvent, leaving group and substrate structure. S_N1, S_N2, S_N1^1, S_N2^1, S_Ni reactions. Neighbouring group participation. Non-classical carbocations. Elimination reactions leading to C=C ond formation and their mechanisms. E1, E2 and E1CB mechanisms. Stereoaspects
of C=C bond formation. Effect of leaving group and substrate structure. Hoffmann and Saytzeff elimination. Cis elimination. Competition between $S_N^1$ and $S_N^2$, E1 and E2, Alkyl halides as survival compounds

**Unit IV Reactivity of unsaturated systems**

18 h


**Unit V Separation techniques**

18 h


**References**


CL 213 PHYSICAL CHEMISTRY -I

Total 90 h

Unit I Quantum Mechanics 18 h


Application to simple systems: Solution of Schrodinger wave equation for a free particle, particle on a ring, particle in 1D box, particle in 3D box, separation of variables, degeneracy.

One dimensional Harmonic oscillator- Complete solution. Hermite polynomials, recursion formula, features of the wave functions.


**Unit II Molecular symmetry** 18 h


Reduction formula, reduction of reducible representation to IRs. Transformation properties of atomic orbitals. Hybridisation: identification of atomic orbitals taking part in hybridisation of triangular planar, square planar, triagonal bipyramidal, square pyramidal and tetrahedral molecules. Molecular symmetry and optical activity.

**Unit III Basics of Chemical Thermodynamics** 18 h


Reaction Isotherm and spontaneity of reaction. Variation of Equilibrium constant with temperature and pressure. Variation of standard free energy with temperature. Simultaneous equillibria and addition of free energies. Standard free energy of formation and its determination, Free energy functions.

**Unit IV Chemical Kinetics 18 h**


Theories of Reaction rate : Arrhenius equation and its limitations, activation energy, Collision theory and absolute reaction rate theory. Free energy of activation and volume of activation. Thermodynamic formulation of reaction rate. Effects of pressure and volume on the velocity of gas reaction.


Unit V  Gases, liquids and liquid crystals  18 h


Liquid crystals: Mesomorphic state, types, examples and applications of liquid crystals. Theory of liquid crystals.

References

1  I.N. Levin, “Quantum Chemistry”, Prentice Hall
5  T. Angel, “Quantum Chemistry and Spectroscopy”, Pearson Education.
6  P. W. Atkins, R.S. Friedman, ”Molecular Quantum Mechanics”, Oxford University Press.
8  F.A. Cotton,” Chemical Applications of Group Theory”, Wiley Eastern


14 S. Glastone, “Thermodynamics for Chemists”,


CL 214 INORGANIC CHEMISTRY PRACTICALS -1

Total 125 h

1. Separation and identification of rare/less familiar cations such as Ti, W, Mo, Th, Zr, V, U and Li

2. Volumetric estimation using EDTA, ammonium vanadate, ceric sulphate etc.

3. Colorimetric/spectrophotometric estimation of Cr, Fe, Mn, Ni, Cu etc.
4. Preparation of metal complexes: selection can be made from the following or any other from the existing literature.

   ii) \([\text{Co(NH}_3\text{)}_6]\text{Cl}_3\), (ii) \([\text{Cu(NH}_3\text{)}_4]\text{SO}_4\) (iii) \(\text{K}_3[\text{Cr(C}_2\text{O}_4\text{)}_3]\)

   iv). \(\text{K}_3[\text{Fe(C}_2\text{O}_4\text{)}_3]\), v). Cis and trans isomers of \([\text{Co(en)}_2\text{Cl}_2]\text{Cl}\)

   iv). \([\text{Cr(en)}_3]\text{Cl}_3\)

References


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**CL 215 ORGANIC PRACTICALS-1**

**Total 125 h**

**A. Separation and identification of organic compounds**

1. Quantitative wet chemistry separation of a mixture of two components by solvent extraction

2. Purification of the separated samples by boiling and crystallization.

3. TLC of the purified samples along with the mixture in same TLC plates (if not possible use separate plates) and calculation of \(R_f\) values.

**B. Separation of a mixture of by column chromatography**

1) Malachite green and methylene blue 2) O-nitroaniline and p-nitroaniline.

**C. Preparation of compounds by two stages.**
TLC analysis of the products and original compound in the same plate and measurement of Rf values. Recording UV, IR, NMR and mass spectrum of synthesized compounds.

1) Acetanilide- → p-nitroacetanilide → p-nitroaniline

2) Methylbenzoate → m-nitromethylbenzoate → m-nitrobenzoic acid

3) Acetanilide- → p-bromoacetanilide → p-bromooaniline

E. Green Organic Chemistry experiments

1) Acetanilide- → p-bromoacetanilide (KBr and CAN)

2) Benzophenone → Benzopinacol (photoreduction)

References


3. Vishnoi, Practical Organic Chemistry, Vikas


5. F G Mann and BC saunders, Practical Organic Chemistry, Pearson


7. C.E Bella and DF Taber, Organic Chemistry Laboratory, Thomson

8. Nelson Practical Biochemistry, Wiley


10. P.D.L Lampman and Chriz, Introduction to Organic Laboratory Techniques, College publishing,

11. Monograph on green laboratory experiments, DST , Govt of India.

12. http://s dbs.riodb.aist.go.jp/s dbs/cgi-bin/direct_frame_top.cgi
CL 216 PHYSICAL PRACTICALS –I

Total 125 h

1. **Adsorption**

Freundlich and Langmuir isotherms for adsorption of acetic/oxalic acid on active charcoal.

Determination of concentration of acetic/oxalic acid.

2. **Kinetics**

Determination of rate constant of acid hydrolysis of methyl acetate.

Determination of Arrhenius parameters.

Determination of concentration of given acid.

Determination of rate constant of the saponification of ethyl acetate and evaluation of Arrhenius parameters.

Determination of rate constant of reaction between $K_2S_2O_8$ and KI.

Study the kinetics of iodination of acetone in acid medium.

3. **Phase rule**

**Solid-liquid equilibria** – Construction of phase diagram and determination of the composition of unknown mixture (naphthalene/biphenyl, naphthalene/benzophenone, naphthalene/diphenyl amine)

Construction of phase diagram with congruent melting point- naphthalene/meta-dinitrobenzene

4. **Partially miscible liquid pairs**- CST of phenol-water system.

Effect of impurities (KCl/NaCl/succinic acid) on the miscibility temperature of phenol-water system and hence the concentration of given unknown solution.

Three component system- Construction of ternary phase diagram of acetic acid-chloroform-water system and hence the composition of given homogeneous mixture.
Construction of tie-line.

5. Distribution law

Distribution coefficient of iodine between CCl₄ and water

Distribution coefficient of benzoic acid between toluene and water.

Determination of the equilibrium constant of the reaction KI+I₂ →[KI₃] and hence the concentration of given KI.

Distribution coefficient of ammonia between chloroform and water.

Determination of equilibrium constant of copper-ammonia complex by partition method or coordination number of Cu²⁺ in copper-ammonia complex.

Determination of hydrolysis constant of anilinium hydrochloride.

6. Dilute Solutions

Determination of Kₓ of solid solvent, molar mass of non-volatile solute, mass of solvent and composition of given solution (Solvent- Naphthalene/Biphenyl/Benzophenone etc. Solute- Naphthalene/Biphenyl/Diphenylanmine etc)

Determination of vant Hoff’s factor for benzoic acid in Naphthalene.

Determination of atomicity of sulphur.

7. Transition temperature

Determination of Kₓ of salt hydrate, molar mass of solute, mass of salt hydrate and composition of given solution (Solvent- Na₂S₂O₃.5H₂O/CH₃COONa.3H₂O, Solutes-glucose, sucrose, urea)

8. Thermochemistry

Determination of the concentration of given strong acid/alkali.

Thermometric titration of NaOH Vs standard HCl.

Heat of displacement of Cu²⁺ by Zn.
Determination of the heat of ionisation of acetic acid.

References


4) A.M.James, and F.E.Pichard, “Practical Physical Chemistry”, Longman.


6) B. Viswanathan, “Practical Physical Chemistry”, Viva Publications.


SEMESTER II

CL 221 INORGANIC CHEMISTRY –II

Unit I  Sulphur, nitrogen, phosphorus and boron compounds  18 h

Sulphur-nitrogen compounds: Tetrasulphur tetranitride, disulphur dinitride and polythiazyl $S_xN_y$ compounds. S-N cations and anions. Other S-N compounds. Sulphur-phosphorous compounds:

Molecular sulphides such as $P_4S_3$, $P_4S_7$, $P_4S_9$ and $P_4S_{10}$. Phosphorous-nitrogen compounds: Phosphazines. Cylco and linear phosphazines. Other P-N compounds

Unit II Coordination Chemistry-II: Spectral and magnetic properties of transition metal complexes 18 h

Electronic spectra of metal complexes- Term symbols of $d^n$ system, Racah parameters, splitting of terms in octahedral and tetrahedral fields. Correlation diagrams for $d^n$ and $d^{10-n}$ ions in octahedral and tetrahedral fields (qualitative approach), $d-d$ transition, selection rules for electronic transition-effect of spin orbit coupling and vibronic coupling

Interpretation of electronic spectra of complexes- Orgel diagrams, Tanabe-Sugano diagrams, Calculation of $Dq$, $B$ and $\beta$ (Nephelauxetic ratio) values, charge transfer spectra.


Unit III Crystalline state 18 h


**Unit IV Lanthanides and actinides** 18 h


**Unit V Solid state chemistry** 18 h


Intrinsic and extrinsic semiconductors, doping of semiconductors and conduction mechanism, the band gap, temperature dependence of conductivity, carrier density and carrier mobility in semiconductors, synthesis and purification of semiconducting materials, single crystal growth, zone refining, fractional crystallization, semiconductor devices, rectifier transistors, optical devices, photoconductors, photovoltaic cells, solar batteries.

**References**

5. J. C. Bailer, ‘Chemistry of Coordination Compounds’, Reinhold.

**CL 222 ORGANIC CHEMISTRY- 11**

**Unit I Molecular rearrangement and transformation reactions** 18 h

Types of organic rearrangements. Anionic, cationotropic, prototropic, free radical, carbene, nitrene and long-range rearrangements. Mechanism with evidence of Wagner-Meerwein, Pinacol, Demjanov, Hofmann, Curtius, Schmidt, Lossen, Beckmann, Wolf, Fries,

**Unit II Aromaticity and symmetry controlled reactions** 18 h


**Unit III Organic photochemistry** 18 h


**Unit IV Chemistry of natural products and biomolecules** 18 h

Introduction to primary and secondary metabolites in plants. Extraction methods of chemical constituents from plants, such as fractionation using solvents, specific extraction of alkaloids and supercritical fluid extraction. Characterizations of isolated compounds (terpenes, sterols, alkaloids, carbohydrates, flavonoids and poly phenols) by colour reactions and spray reagents. Biosynthesis of terpenes from mevalonic acid and sterols from squalene. Structure elucidation of ocimene monoterpene, classification of pigments, structure elucidation of β –carotene. Structural differences between a triterpene and a sterol. Synthesis of quercetin, synthesis of testosterone, androsterone, estrone and progesterone. Determination of carbon skeleton of alkaloids (Hofmann, Emde and Von Braun degradation methods). Structural elucidation of ephedrine, nicotine, atropine, hygrine.

**Unit V Physical organic chemistry** 18 h

References

1. L.M. Harwood, Polar rearrangements, Oxford University.
5. P.Y. Bruice, Organic chemistry, Prentice Hall.
12. R.J. Simmonds, Chemistry of Biomolecules, Royal Society of Chemistry.
13. J. Mann and others, Natural products- Their Chemistry and Biological Significance, Longmann
16. N.R. Krishnaswamy, Chemistry of Natural Products, A Unified Approach.
17. N. R. Krishnaswamy, Chemistry of Natural Products, A llaboratory Hand Book.
18. J.B. Harborne, Phytochemical Methods, Chapman and Hall.
CL 223 PHYSICAL CHEMISTRY -II

Unit I  Chemical Bonding  18 h


Perturbation method-Successive correction to an unperturbed problem. Detailed treatment of first order non-degenerate case only. LCAO-MO Theory- MO theory of $H_2^+$ and $H_2$. MO treatment of other homo diatomic molecules Li$_2$, Be$_2$, B$_2$, C$_2$, N$_2$, O$_2$ and F$_2$. MO treatment of hetero diatomic molecules LiH, CO, NO and HF. Spectroscopic term symbols for homo diatomic molecules.

Valence bond theory of $H_2$. Quantum mechanical treatment of SP, SP$^2$ and SP$^3$ Hybridisation.

HMO theory of conjugated $\pi$-systems. Bond order and charge density calculations. Free valance. Application of HMO method to ethylene, allyl system, butadiene and benzene.

Secondary bond forces: ion dipole, dipole-dipole, ion-induced dipole, London dispersion forces.

Unit II  Spectroscopy –I  18 h

Microwave spectroscopy: Rotational spectrum, Intensity of spectral lines, calculation of inter nuclear distance. Non-rigid rotors and centrifugal distortion. Rotational spectra of polyatomic molecules-linear and symmetric top molecules. Introduction to instrumentation.


Vibrational spectra of polyatomic molecules: Normal modes, classification of vibrational modes into stretching (asymmetric, symmetric), bending, parallel and perpendicular
vibrations. Finger print region and group frequencies. Introduction to FTIR and instrumentation.


**Unit III Applications of thermodynamics**

Phase equilibria: Criteria of Equilibrium. Derivation of phase rule Discussion of two component systems forming solid solutions with and without maximum or minimum in freezing point curve. Systems with partially miscible solid phases.


Unit IV Statistical mechanics –I  


The Partition functions. Partition function for free linear motion, for free motion in a shared space, for linear harmonic vibration.

Unit V Electrochemistry  


Fuel cells- H₂-O₂ fuel cell, fuel cell for high temperature applications.

References

1  I.N. Levine, “Quantum Chemistry”, Printice Hall.
14 C. Kalidas, M. V. Sangaranarayanan, “Non-equilibrium Thermodynamics”, Macmillan India.
15 McQuarrie, “Statistical Mechanics”, Orient Longman.
18 S. Glasstone, “Introduction to Electrochemistry”,
SEMESTER III

CL. 231 INORGANIC CHEMISTRY- III

Total 90 h

Unit I Organometallic compounds 18 h


Unit II Coordination chemistry-III: Reactions of metal complexes 18 h

Energy profile of a reaction - Thermodynamic and kinetic stability, Classification of ligand substitution reactions - kinetics and mechanism of ligand substitution reactions in square planar complexes, trans effect- theory and synthetic applications.

Kinetics and mechanism of octahedral substitution- water exchange, dissociative and associative mechanisms, base hydrolysis, racemization reactions, solvolytic reactions (acidic and basic)


Unit III Bioinorganic chemistry 18 h

Essential and trace elements in biological systems, structure and functions of biological membranes, mechanism of ion transport across membranes, sodium-potassium
pump. Photosynthesis, porphyrin ring system, chlorophyll, PS I and PS II. Synthetic model for photosynthesis. Role of calcium in biological systems.


**Unit IV Electrical and magnetic properties of solids** 18 h


**Unit V Nuclear chemistry** 18 h


References

Unit 1 UV-VIS, IR and Mass spectroscopy  

Unit II NMR spectroscopy and structure elucidation  
Theory of NMR spectroscopy, chemical shifts, anisotropic effects and coupling constant. Spin-spin interactions in typical systems. First order and second order spectra. Simplification methods of complex spectra by high field NMR, shift reagents, chemical exchange and doule resonance. Theories of FT NMR (1D NMR), 2D NMR and $^{13}$C NMR spectroscopies. $^{13}$C NMR chemical shifts. Instrumentation of NMR. Applications of NOE, APT, DEPT, INEPT and 2-DNMR and INADEQUATE, HOHA spectroscopies. Introduction to 3D NMR. Spectral interpretations and structure identification. Spectral interpretation using actual spectra taken from standard texts. Solving of structural problems on the basis of numerical and spectrum based data.

Unit III Molecular recognition and supramolecular chemistry  

Unit IV Medicinal chemistry 18 h

Retrosynthetic analysis and disconnection approach. Synthetic strategy and synthons.

Combinatorial organic synthesis, introduction, methodology, automation, solid supported and solution phase synthesis, study of targeted or focused libraries and small molecule libraries. Application- drug discovery.


Unit V Green chemistry 18 h


References


5. H.O. House, Modern synthetic reactions, Benjamin Cummins.


9. R.M. Merhotra and Singh, Organometallic chemistry.


11. J.M. Lehn, Supramolecular chemistry, VCH.


13. V.K. Ahluwalia and Mahu Chopra, Medicinal chemistry.


15. Ashutosh Kar, Medicinal chemistry.


17. P.Y. Bruice, Organic chemistry, Prentice Hall.

18. P.T. Anastas, and J.C. Warner, Green chemistry, Theory and Practice, OUP.


Unit I Computational chemistry. 18 h

Introduction to computational chemistry, concept of potential energy surface (PES), stationary point, saddle point and geometry optimisation.

Basis sets, STO, Gaussian functions and its properties, GTO, contracted Gaussians, minimal, split valance, polarised and diffused basis sets.

Introduction to SCF. Wave function for open shell state, RHF, ROHF and URHF. Model Chemistry. Brief description of computational methods- ab-initio, semiempirical and density functional and molecular mechanics methods. Construction of Z-matrix for simple molecules- H₂O, H₂O₂, H₂CO, CH₃CHO, NH₃, and CO₂.

Unit II Spectroscopy II 18 h


ESR spectroscopy: Electron spin. Interaction with magnetic field. Kramer’s rule. The g factor. Determination of g values. Fine structure and hyperfine structure. Elementary idea of ENDOR and ELDOR.


Photoelectron spectroscopy. Introduction to UV photoelectron and X-ray photoelectron spectroscopy.

Unit III Statistical mechanics II 18 h

Complex partition functions and partition function for particles in different force fields. Langevin’s partition function and its use for the determination of dipole moment. Electrostatic energies. Molecular partition functions. Translational, vibrational, rotational and electronic partition functions. Total partition functions, partition functions and


Unit IV Surface chemistry and catalysis


Surface films: different types, Surface pressure and Surface potential, and their measurements and interpretation.


Catalysis: Mechanism and theories of homogeneous and heterogeneous catalysis. Enzyme catalysis, Bimolecular surface reactions. Langmuir – Hinshelwood mechanism
Instrumental methods of catalyst characterization- diffraction and thermal methods, spectroscopic and microscopic techniques.

**Unit V Electro Analytical and spectrophotometric methods.**

18 h


Flame emission and atomic absorption spectrometry. Instrumentation for AAS. The flame characteristics. Atomiser used in spectroscopy. Hollow cathode lamp. Interference in AAS. Application of AAS.

**References**


11 G.A. Somorjai. Y. Li, Introduction to Surface Chemistry and Catalysis.


14 McQuarrie, “Statistical Mechanics”, Orient Longman

15 G.W. Castellan, ”Physical Chemistry”, Addison-Lesley Publishing.

16 P.W. Atkins, ”Physical Chemistry”, Oxford University Press.


18 D. Chandler. Introduction to Modern Statistical Mechanics, Oxford University Press.


CL 234 Inorganic Chemistry Practicals -II Total-125 h

1. Estimation of simple mixture of ions (involving quantitative separation) by volumetric and Gravimetric methods.

2. Analysis of typical alloys and ores

3. Ion exchange separation of binary mixtures.

4. Spectral Interpretation of metal complexes using IR, UV-Vis. spectral data. Supplementary information like metal estimation, CHN analysis, conductivity measurements and magnetic measurements to be provided to the students. Assessment is based on arriving at the structure of the complex and assignment of IR spectral bands.

5. Interpretation of TG and DTA curves of metal oxalates/acetates/sulphates/chlorides in hydrated forms. Assessment is based on the identification of various stages.
References

4. Willard, Merrit and Dean, ‘Instrumental Methods of Analysis,’

CL 235 ORGANIC PRACTICALS-II

Total 125 h

A. Volumetric estimation of
   1) Aniline  2) Phenol  3) glucose
   4) Iodine value and saponification value of coconut oil


C). Spectral identification (UV, IR, $^1$H NMR, $^{13}$C NMR, EI mass) of Organic compounds from a library of organic compounds

D. Separations of mixtures by Paper Chromatography

1) Separation of amino acids  2) Separation of dyes

E) Three stage preparation

1) Benzaldehyde $\rightarrow$ Benzoin( green synthesis with thiamine HCl) $\rightarrow$ benzil
benzilic acid

2) Phthalic acid → Phthalic anhydride → pthalimide → anthranilic acid

References

3. Vishnoi, Practical Organic Chemistry, Vikas
4. R.M Silverstein, Spectrometric identification of Organic compounds
5. F G Mann and BC saunders, Practical Organic Chemistry, Pearson
7. C.E Bella and DF Taber, Organic Chemistry laboratory, Thomson
8. Nelson Practical Biochemistry, wiley
10. P.D.L Lampman and Chriz, Introduction to organic Laboratory techniques, College publishing,
11. Monograph on green laboratory experiments, DST , Govt of India.
12. http://sdbl.riodb.aist.go.jp/sdbs/cgi-bin/direct_frame_top.cgi

CL 236 PHYSICAL PRACTICALS –II  Total 125 h

1. Conductometry

Determination of strength of strong and weak acids in a mixture
Determination of strength of a weak acid.
Determination of solubility product of a sparingly soluble salt (PbSO₄, BaSO₄ etc.)
Hydrolysis of NH₄Cl or CH₃COONa or aniline hydrochloride
Determination of order of reaction, rate constant and energy of activation for saponification of ethyl acetate
Precipitation titrations.
Determination of critical micellar concentration (CMC) of sodium lauryl sulphate from
measurement of conductivities at different concentrations.
Equivalent conductance at infinite dilutions and verification of Kohlraush’s Law.
Determination of Onsager constants.

2. Potentiometry
Determination of emf of Daniel cell.
Determination of the emf of various ZnSO₄ solutions and hence the concentration of unknown ZnSO₄ solution.
Determination of valency of mercurous ion.
Determination of temperature dependence of EMF of a cell
Determination of stoichiometry and formation constant of silver-ammonia complex.
Determination of activity and activity constant of electrolytes.
Determination of thermodynamic constants of reactions.

pH metric titrations.
Acid alkali titrations using Quinhydrone electrode.
Titrations(double) involving redox reactions – Fe²⁺ Vs KMnO₄, K₂Cr₂O₇, Ce(NH₃)SO₄ and KI Vs KMnO₄
Determination of strengths of halides in a mixture.
Determination of pH of buffer solutions and hence to calculate the E₀ of quinhydrone electrode

3. Spectrophotometry
Verification of Beer-Lambert’s law.
Absorption spectra of conjugated dyes.
Determination of concentration of potassium dichromate and potassium permanganate in a mixture.
To study the complex formation between Fe³⁺ and salicylic acid.
Determination of pKa of an indicator.

4. Polarimetry
Measurement specific rotation of glucose.
Determination of specific rotation of sucrose
Determination of unknown concentration of glucose solution.
and rate constant of its hydrolysis in presence of HCl
Polarography:
Determination of half wave potential $E_{1/2}$ and unknown concentration of Cd$^{2+}$ ion.
Determination of concentrations of metal ions in a mixture.

5. Surface tension
Determination of surface tension of various liquids by Stalagmometric method (drop number / drop weight)
Determination of parachors of molecules and various groups.
Determination of concentration of a mixture.
Determination of surface tension and parachor of liquids using double capillary method.

6. Refractometry
Determination of molar refraction of pure liquids
Determination of concentration of KCl solution/glycerol solution
Determination of solubility of KCl in water.
Determination of molar refraction of solid KCl
Study the stoichiometry of potassium iodide-mercuric iodide complex.
Determination of concentration of KI solution.

7. Viscosity
Determination of viscosity of various liquids using Ostwald’s viscometer.
Determination of unknown composition of given liquid mixture like toluene-nitrobenzene.
Verification of Kendall’s relation.
Verification of Jon Dole’s equation.

References
B. P. Levitt and J.A. Kitchener,”Findlay's Practical Physical Chemistry”,
Longmans, London.
A.M.James, and F.E. Pichard, “Practical Physical Chemistry”, Longman.
B. Viswanathan, “Practical Physical Chemistry”, Viva Publications.
SEMESTER IV

Total 90 h

CL 241 APPLIED ANALYTICAL CHEMISTRY

Unit I Water and wastewater analysis 18 h


Unit II Soil analysis 18 h


Unit III Air pollution analysis  18 h


Unit IV Food and forensic analyses:  18 h

Moister, 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. Special features of Forensic analysis, sampling, sample storage, sample dissolution, classification of poisons, Lethal dose, significance of LD 50 and LC 50. Identification and Analysis in the suspects: Poisonous elements viz As, Sb, Pb, Cr and Hg. Insecticides Analysis of metals, Gun powder Residues, portland cement in Forensic samples. Poisoning due to cyanide, dioxines & asbestos. Physiological effects of natural poisons such as Col Chicine, Morphine, Hashish, Nicotinoids. Health hazards and Remedial measures.

Unit V Analysis of selected materials  18 h


REFERENCES


• “British Pharmacopoeia”, Her Majesty's Stationery Office, 1988


• S.M. Khopkar, “Environmental Pollution Analysis”. New Age International (P) Ltd.


• B.J. Alloway and D.C. Ayres, “Chemical Principles of Environmental Pollution”. Blackie Academic & Professional, 1997


**CL 242 DISSERTATION**

Each of the students has to carry out original research in a topic in accordance with the Elective paper chosen for Semester IV under the guidance and supervision of a teacher in the concerned Department of the College.

Instructions to Question Papers Setters

The Syllabus of each theory has five units. While setting the question papers, equal weight is to be given to each of the Units for choosing the questions. Each question paper is of 3 hours duration and has three Sections, namely Section A, Section B and Section C constituting a total 75 marks as detailed.
Section A Five questions, one from each Unit containing three short answer questions marked (a), (b), and (c), each of which has 2 marks. One has to answer any two of (a), (b) or (c) from each of the five questions. (2x10=20 marks)

Section B Five questions, one from each Unit containing two short essay questions marked (a) and (b), each of which has marks. One has to answer either (a) or (b) from each of the five questions. (5x5=25 marks)

Section C Five essay questions, one from each unit having 10 marks. One has to answer any three questions from the five questions asked. (1x3=30 marks).
### M.Sc. PROGRAMME IN BRANCH V – APPLIED CHEMISTRY

(Revised syllabus under semester system with effect from 2013 admission)

**SYLLABUS AND SCHEME OF EXAMINATION**

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<th>Hours per week</th>
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*Distribution of teaching hours/week: Theory- 15 hours, Practicals- 10 hours (1 hour for Seminar)*

| **SEMESTER II***                     |                |                          |              |               |             |
| CA 221 Inorganic Chemistry II        | 5              | 3                        | 25           | 75            | 100         |
| CA 222 Organic Chemistry II          | 5              | 3                        | 25           | 75            | 100         |
| CA 223 Physical Chemistry II         | 5              | 3                        | 25           | 75            | 100         |
| CA 214 Inorganic Practicals I        | 3              | 6                        | 25           | 75            | 100         |
| CA 215 Organic Practicals I          | 3              | 6                        | 25           | 75            | 100         |
| CA 216 Physical Practicals I         | 4              | 6                        | 25           | 75            | 100         |
| Total marks for Semester II          |                |                          |              |               | 600         |

*Distribution of teaching hours/week: Theory- 15 hours, Practicals- 10 hours (1 hour for Seminar)*
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*Distribution of teaching hours/week: Theory- 15 hours, Practicals- 10 hours (1 hour for Seminar)

| Total marks for semester III | 300 |

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| Total marks for Semester IV | 600 |
| Grand total (for semesters I-IV) | 1800 |

*Distribution of teaching hours/week: Theory- 15 hours, 10 hours for discussion on project (1 hour for Seminar)
M.Sc. PROGRAMME IN BRANCH V – APPLIED CHEMISTRY
(Revised syllabus under Semester System w.e.f. 2013 Admission)

SEMESTER I

CA 211 INORGANIC CHEMISTRY - I

Total 90 h

Unit I  Noble gases, halogens, isopoly and heteropoly acids  18 h

Noble gas compounds: Preparation, properties, structure and bonding. Halogens in positive oxidation states. Preparation, properties, structure, bonding and uses of inter halogen compounds, pseudo halogens, poly halide ions. Astatine: Synthesis, stability and properties.

Preparation, properties and structure of isopoly and heteropoly acids of Mo and W. Classification, preparation, properties and structure of borides, carbides, nitrides and silicides. Classification and structure of silicates. Properties and structure of aluminosilicates and zeolites. Preparation, properties and applications of silicones.

Unit II  Coordination chemistry-I: Theories of metal complexes  18 h


Unit III Analytical principles 18 h


Unit IV Nanomaterials 18 h

General introduction to nanomaterials and emergence of nanotechnology, Moore’s law, synthesis and properties of fullerenes and carbon nanotubes, synthesis of nanoparticles of gold, silver, rhodium, palladium and platinum. Techniques of synthesis- electroplating and electrophoretic deposition, conversion through chemical reactions and lithography. Thin films- chemical vapour deposition and atomic layer deposition techniques.

Elementary idea of characterization of nanomaterials using XRD powder, TEM, AFM, SEM and STM techniques.


Unit V Chemistry of natural environmental processes 18 h.


References

15. C.P. Poole Jr. and J. Owens, ‘Introduction to Nanotechnology,’ Wiley India.
17. H.V. Jadhav, Elements of Environmental Chemistry.

CA 212 ORGANIC CHEMISTRY - I

Unit I Stereochemistry of organic compounds 18 h

Nomenclature of organic compounds, Fused polycyclic hydrocarbons, Bridged polycyclic hydrocarbons, Bridged fused systems, Spirocyclic hydrocarbon systems, Heterocyclic systems, Metal organic compounds.


Unit II Structure, reactivity and intermediates 18 h


Unit III. Substitution and elimination reactions 18 h

Nucleophilic susbtitution at sp3 carbon, its mechanisms and stereochemical aspects. Effect of solvent, leaving group and substrate structure. S_N1, S_N2, S_N1, S_N2, S_N reactions. Neighbouring group participation. Non-classical carbocations. Elimination reactions leading to C=C ond formation and their mechanisms. E1, E2 and E1CB mechanisms. Stereoaspects
of C=C bond formation. Effect of leaving group and substrate structure. Hoffmann and Saytzeff elimination. Cis elimination. Competition between \( S_N^1 \) and \( S_N^2 \), E1 and E2. Alkyl halides as survival compounds

**Unit IV Reactivity of unsaturated systems**

18 h


**Unit V Separation techniques**

18 h


**References**


CA 213 PHYSICAL CHEMISTRY -I

Total 90 h

Unit I Quantum mechanics 18 h


Application to simple systems: Solution of Schrödinger wave equation for a free particle, particle on a ring, particle in 1D box, particle in 3D box, separation of variables, degeneracy.

One dimensional Harmonic oscillator- Complete solution. Hermite polynomials, recursion formula, features of the wave functions.


Unit II Molecular symmetry


Reduction formula, reduction of reducible representation to IRs. Transformation properties of atomic orbitals. Hybridisation: identification of atomic orbitals taking part in hybridisation of triangular planar, square planar, triagonal bipyramidal, square pyramidal and tetrahedral molecules. Molecular symmetry and optical activity.

Unit III Basics of chemical thermodynamics


Reaction Isotherm and spontaneity of reaction. Variation of Equilibrium constant with temperature and pressure. Variation of standard free energy with temperature. Simultaneous equillibria and addition of free energies. Standard free energy of formation and its determination, Free energy functions.

Unit IV Chemical kinetics


Theories of Reaction rate: Arrhenius equation and its limitations, activation energy, Collision theory and absolute reaction rate theory. Free energy of activation and volume of activation. Thermodynamic formulation of reaction rate. Effects of pressure and volume on the velocity of gas reaction.


Unit V  Gases, liquids and liquid crystals  18 h


Liquid crystals: Mesomorphic state, types, examples and applications of liquid crystals. Theory of liquid crystals.

References

1  I.N. Levin, “Quantum Chemistry”, Prentice Hall
5  T. Angel, “Quantum Chemistry and Spectroscopy”, Pearson Education.
6  P. W. Atkins, R. S. Friedman, ”Molecular Quantum Mechanics”, Oxford University Press.
8  F. A. Cotton,” Chemical Applications of Group Theory”, Wiley Eastern


14 S.Glastone, “Thermodynamics for Chemists”,


CA 214 INORGANIC CHEMISTRY PRACTICALS -1

Total 125 h

1. Separation and identification of rare/less familiar cations such as Ti, W, Mo, Th, Zr, V, U and Li

2. Volumetric estimation using EDTA, ammonium vanadate, ceric sulphate etc.

3. Colorimetric/spectrophotomteric estimation of Cr, Fe, Mn, Ni, Cu etc.
4. Preparation of metal complexes: selection can be made from the following or any other from the existing literature.

iii) $[\text{Co(NH}_3\text{)}_6]\text{Cl}_3$  (ii). $[\text{Cu(NH}_3\text{)}_4]\text{SO}_4$  (iii) $K_3[\text{Cr(C}_2\text{O}_4\text{)}_3]$  

iv). $K_3[\text{Fe(C}_2\text{O}_4\text{)}_3]$, v). Cis and trans isomers of $[\text{Co(en)}_2\text{Cl}_2]\text{Cl}$  

iv). $[\text{Cr(en)}_3]\text{Cl}_3$

References


CA 215 ORGANIC PRACTICALS-1

Total 125 h

A. Separation and identification of organic compounds

1. Quantitative wet chemistry separation of a mixture of two components by solvent extraction

2. Purification of the separated samples by boiling and crystallization.

3. TLC of the purified samples along with the mixture in same TLC plates (if not possible use separate plates) and calculation of $R_f$ values.

B. Separation of a mixture of by column chromatography

1) Malachite green and methylene blue 2) O-nitroaniline and p-nitroaniline.

C. Preparation of compounds by two stages.
TLC analysis of the products and original compound in the same plate and measurement of Rf values. Recording UV, IR, NMR and mass spectrum of synthesized compounds.

1) Acetanilide → p-nitroacetanilide → p-nitroaniline
2) Methylbenzoate → m-nitromethylbenzoate → m-nitrobenzoic acid
3) Acetanilide → p-bromoacetanilide → p-bromooaniline

E. Green Organic Chemistry experiments

1) Acetanilide → p-bromoacetanilide (KBr and CAN)
2) Benzophenone → Benzpinacol (photoreduction)

References

3. Vishnoi, Practical Organic Chemistry, Vikas
5. F G Mann and BC saunders, Practical Organic Chemistry, Pearson
7. C.E Bella and DF Taber, Organic Chemistry Laboratory, Thomson
8. Nelson Practical Biochemistry, Wiley
10. P.D.L Lampman and Chriz, Introduction to Organic Laboratory Techniques, College publishing.
11. Monograph on green laboratory experiments, DST , Govt of India.
12. http://s dbs.riodb.aist.go.jp/sdbs/cgi-bin/direct_frame_top.cgi
1. adsorption

Freundlich and Langmuir isotherms for adsorption of acetic/oxalic acid on active charcoal.

Determination of concentration of acetic/oxalic acid.

2. kinetics

Determination of rate constant of acid hydrolysis of methyl acetate.

Determination of Arrhenius parameters.

Determination of concentration of given acid.

Determination of rate constant of the saponification of ethyl acetate and evaluation of Arrhenius parameters.

Determination of rate constant of reaction between $\text{K}_2\text{S}_2\text{O}_8$ and KI.

Study the kinetics of iodination of acetone in acid medium.

3. phase rule

**Solid-liquid equilibria** – Construction of phase diagram and determination of the composition of unknown mixture (naphthalene/biphenyl, naphthalene/benzophenone, naphthalene/diphenyl amine)

Construction of phase diagram with congruent melting point - naphthalene/meta-dinitrobenzene

**Partially miscible liquid pairs** - CST of phenol-water system.

Effect of impurities (KCl/NaCl/succinic acid) on the miscibility temperature of phenol-water system and hence the concentration of given unknown solution.

Three component system - Construction of ternary phase diagram of acetic acid-chloroform-water system and hence the composition of given homogeneous mixture.
Construction of tie-line.

4. Distribution law

Distribution coefficient of iodine between CCl₄ and water

Distribution coefficient of benzoic acid between toluene and water.

Determination of the equilibrium constant of the reaction KI+I₂ \( \rightarrow \) [KI₃] and hence the concentration of given KI.

Distribution coefficient of ammonia between chloroform and water.

Determination of equilibrium constant of copper-ammonia complex by partition method or coordination number of Cu²⁺ in copper-ammonia complex.

Determination of hydrolysis constant of anilinium hydrochloride.

5. Dilute Solutions

Determination of Kₐ of solid solvent, molar mass of non-volatile solute, mass of solvent and composition of given solution (Solvent- Naphthalene/Biphenyl/Benzophenone etc. Solute- Naphthalene/Biphenyl/Diphenylanmine etc)

Determination of vant Hoff’s factor for benzoic acid in Naphthalene.

Determination of atomicity of sulphur.

6. Transition temperature

Determination of Kₜ of salt hydrate, molar mass of solute, mass of salt hydrate and composition of given solution (Solvent- Na₂S₂O₃.5H₂O/CH₃COONa.3H₂O, Solutes-glucose, sucrose, urea)

7. Thermochemistry

Determination of the concentration of given strong acid/alkali.

Thermometric titration of NaOH Vs standard HCl.

Heat of displacement of Cu²⁺ by Zn.
Determination of the heat of ionisation of acetic acid.

References

2) B. P. Levitt and J.A. Kitchener, ”Findlay's Practical Physical Chemistry”, Longmans, London.
4) A. M. James, and F. E. Pichard, “Practical Physical Chemistry”, Longman.
6) B. Viswanathan, “Practical Physical Chemistry”, Viva Publications.

SEMESTER II

CA 221 INORGANIC CHEMISTRY –II

Total 90 h

Unit I  Sulphur, nitrogen, phosphorus and boron compounds  18 h

Sulphur-nitrogen compounds: Tetrasulphur tetranitride, disulphur dinitride and polythiazyl S\textsubscript{x}N\textsubscript{y} compounds. S-N cations and anions. Other S-N compounds. Sulphur-phosphorous compounds:

Molecular sulphides such as P\textsubscript{4}S\textsubscript{3} , P\textsubscript{4}S\textsubscript{7} , P\textsubscript{4}S\textsubscript{9} and P\textsubscript{4}S\textsubscript{10} . Phosphorous-nitrogen compounds: Phosphazines. Cylco and linear phosphazines. Other P-N compounds

**Unit II Coordination chemistry-II: Spectral and magnetic properties of transition metal complexes**  
18 h

Electronic spectra of metal complexes- Term symbols of $d^n$ system, Racah parameters, splitting of terms in octahedral and tetrahedral fields. Correlation diagrams for $d^n$ and $d^{10-n}$ ions in octahedral and tetrahedral fields (qualitative approach), $d$-$d$ transition, selection rules for electronic transition-effect of spin orbit coupling and vibronic coupling

Interpretation of electronic spectra of complexes- Orgel diagrams, Tanabe-Sugano diagrams, Calculation of $Dq$, $B$ and $\beta$ (Nephelauxetic ratio) values, charge transfer spectra.


**Unit III Crystalline state**  
18 h


**Unit IV Lanthanides and actinides**


**Unit V Solid state chemistry**


Intrinsic and extrinsic semiconductors, doping of semiconductors and conduction mechanism, the band gap, temperature dependence of conductivity, carrier density and carrier mobility in semiconductors, synthesis and purification of semiconducting materials, single crystal growth, zone refining, fractional crystallization, semiconductor devices, rectifier transistors, optical devices, photoconductors, photovoltaic cells, solar batteries.

**References**

5. J. C. Bailar, ‘Chemistry of Coordination Compounds’, Reinhold.

CA 222 ORGANIC CHEMISTRY- 11

Total 90 h

Unit I Molecular rearrangement and transformation reactions 18h

Types of organic rearrangements. Anionic, cationotropic, prototropic, free radical, carbene, nitrene and long-range rearrangements. Mechanism with evidence of Wagner-Meerwein, Pinacol, Demjanov, Hofmann, Curtius, Schmidt, Lossen, Beckmann, Wolf, Fries,

Unit II Aromaticity and symmetry controlled reactions 18 h


Unit III Organic photochemistry 18 h


Unit IV Chemistry of natural products and biomolecules 18 h

Introduction to primary and secondary metabolites in plants. Extraction methods of chemical constituents from plants, such as fractionation using solvents, specific extraction of alkaloids and supercritical fluid extraction. Characterizations of isolated compounds (terpenes, sterols, alkaloids, carbohydrates, flavonoids and poly phenols) by colour reactions and spray reagents. Biosynthesis of terpenes from mevalonic acid and sterols from squalene. Structure elucidation of oicmene monoterpen, classification of pigments, structure elucidation of β –carotene. Structural differences between a triterpene and a sterol. Synthesis of quercetin, synthesis of testosterone, androsterone, estrone and progesterone. Determination of carbon skeleton of alkaloids (Hofmann, Emde and Von Braun degradation methods). Structural elucidation of ephedrine, nicotine, atropine,hygrine.

Unit V Physical organic chemistry 18 h

References

1. L.M. Harwood, Polar rearrangements, Oxford University.
5. P.Y. Bruice, Organic chemistry, Prentice Hall.
12. R.J. Simmonds, Chemistry of Biomolecules, Royal Society of Chemistry.
13. J. Mann and others, Natural products- Their Chemistry and Biological Significance, Longmann
16. N.R. Krishnaswamy, Chemistry of Natural Products, A Unified Approach.
17. N. R. Krishnaswamy, Chemistry of Natural Products, A llaboratory Hand Book.
19. J.B. Harborne, Phytochemical Methods, Chapman and Hall.
CA 223 PHYSICAL CHEMISTRY -II

Unit I  Chemical Bonding  18 h

Approximate methods: Variation method- Variation theorem and its proof. Linear variation functions. Secular equations and secular determinants.

Perturbation method-Successive correction to an unperturbed problem. Detailed treatment of first order non-degenerate case only. LCAO-MO Theory- MO theory of $H_2^+$ and $H_2$. MO treatment of other homo diatomic molecules Li$_2$, Be$_2$, B$_2$, C$_2$, N$_2$, O$_2$ and F$_2$. MO treatment of hetero diatomic molecules LiH, CO, NO and HF. Spectroscopic term symbols for homo diatomic molecules.

Valance bond theory of $H_2$. Quantum mechanical treatment of SP, SP$^2$ and SP$^3$ Hybridisation.

HMO theory of conjugated $\pi$-systems. Bond order and charge density calculations. Free valance. Application of HMO method to ethylene, allyl system, butadiene and benzene.

Secondary bond forces: ion dipole, dipole-dipole, ion-induced dipole, London dispersion forces.

Unit II  Spectroscopy –I  18 h

Microwave spectroscopy: Rotational spectrum, Intensity of spectral lines, calculation of inter nuclear distance. Non-rigid rotors and centrifugal distortion. Rotational spectra of polyatomic molecules-linear and symmetric top molecules. Introduction to instrumentation.


Vibrational spectra of polyatomic molecules: Normal modes, classification of vibrational modes into stretching (asymmetric, symmetric), bending, parallel and perpendicular
vibrations. Finger print region and group frequencies. Introduction to FTIR and instrumentation.


Unit III Applications of thermodynamics

Phase equilibria: Criteria of Equilibrium. Derivation of phase rule Discussion of two component systems forming solid solutions with and without maximum or minimum in freezing point curve. Systems with partially miscible solid phases.


Unit IV  Statistical mechanics –I  


The Partition functions. Partition function for free linear motion, for free motion in a shared space, for linear harmonic vibration.

Unit V Electrochemistry


Fuel cells- H2-O2 fuel cell, fuel cell for high temperature applications.

# References

18. S. Glasstone, “Introduction to Electrochemistry”,
SEMESTER III

CA 231 INORGANIC CHEMISTRY - III

Total 90 h

Unit I Organometallic compounds


Unit II Coordination chemistry-III: Reactions of metal complexes

Energy profile of a reaction - Thermodynamic and kinetic stability, Classification of ligand substitution reactions - kinetics and mechanism of ligand substitution reactions in square planar complexes, trans effect - theory and synthetic applications.

Kinetics and mechanism of octahedral substitution- water exchange, dissociative and associative mechanisms, base hydrolysis, racemization reactions, solvolytic reactions (acidic and basic)

Electron transfer reactions: Outer sphere mechanism- Marcus theory, inner sphere mechanism- Taube mechanism. Photochemical reactions- substitution and redox reactions of Cr(III), Ru(II), and Ru(III) complexes. Photo-isomerisation and photo-aquation reactions of metal complexes.

Unit III Bioinorganic chemistry

Essential and trace elements in biological systems, structure and functions of biological membranes, mechanism of ion transport across membranes, sodium-potassium
pump. Photosynthesis, porphyrin ring system, chlorophyll, PS I and PS II. Synthetic model for photosynthesis. Role of calcium in biological systems.


**Unit IV Electrical and magnetic properties of solids** 18 h


**Unit V Nuclear chemistry** 18 h


Unit I UV-VIS, IR and Mass spectroscopy


Unit II NMR spectroscopy and structure elucidation

Theory of NMR spectroscopy, chemical shifts, anisotropic effects and coupling constant. Spin-spin interactions in typical systems. First order and second order spectra. Simplification methods of complex spectra by high field NMR, shift reagents, chemical exchange and double resonance. Theories of FT NMR (1D NMR), 2D NMR and $^{13}$C NMR spectroscopies. $^{13}$C NMR chemical shifts. Instrumentation of NMR. Applications of NOE, APT, DEPT, INEPT and 2-DNMR and INADEQUATE, HOHA spectroscopies. Introduction to 3D NMR. Spectral interpretations and structure identification. Spectral interpretation using actual spectra taken from standard texts. Solving of structural problems on the basis of numerical and spectrum based data.

Unit III Molecular recognition and supramolecular chemistry


**Unit IV Medicinal chemistry**

18 h

Retroynthetic analysis and disconnection approach. Synthetic strategy and synthons,

Combinatorial organic synthesis, introduction, methodology, automation, solid supported and solution phase synthesis, study of targeted or focused libraries and small molecule libraries, Application- drug discovery.


**Unit V Green chemistry**

18 h


**References**


5. H.O. House, Modern synthetic reactions, Benjamin Cummins.


9. R.M. Merhotra and Singh, Organometallic chemistry.


11. J.M. Lehn, Supramolecular chemistry, VCH.


13. V.K. Ahluwalia and Mahu Chopra, Medicinal chemistry.


15. Ashutosh Kar, Medicinal chemistry.


17. P.Y. Bruice, Organic chemistry, Prentice Hall.

18. P.T. Anastas, and J.C. Warner, Green chemistry, Theory and Practice, OUP.


Unit I Computational chemistry.  18 h

Introduction to computational chemistry, concept of potential energy surface (PES), stationary point, saddle point and geometry optimisation.

Basis sets, STO, Gaussian functions and its properties, GTO, contracted Gaussians, minimal, split valance, polarised and diffused basis sets.

Introduction to SCF. Wave function for open shell state, RHF, ROHF and URHF. Model Chemistry. Brief description of computational methods- ab-initio, semiempirical and density functional and molecular mechanics methods. Construction of Z-matrix for simple molecules- H₂O, H₂O₂, H₂CO, CH₃CHO, NH₃, and CO₂.

Unit II Spectroscopy II  18 h


ESR spectroscopy: Electron spin. Interaction with magnetic field. Kramer’s rule. The g factor. Determination of g values. Fine structure and hyperfine structure. Elementary idea of ENDOR and ELDOR.


Photoelectron spectroscopy. Introduction to UV photoelectron and X-ray photoelectron spectroscopy.

Unit III Statistical mechanics II  18 h

Complex partition functions and partition function for particles in different force fields. Langevin’s partition function and its use for the determination of dipole moment. Electrostatic energies. Molecular partition functions. Translational, vibrational, rotational and electronic partition functions. Total partition functions, partition functions and


Unit IV Surface chemistry and catalysis 18 h


Surface films: different types, Surface pressure and Surface potential, and their measurements and interpretation.


Catalysis: Mechanism and theories of homogeneous and heterogeneous catalysis. Enzyme catalysis, Bimolecular surface reactions. Langmuir – Hinshelwood mechanism

Instrumental methods of catalyst characterization- diffraction and thermal methods, spectroscopic and microscopic techniques.
Unit V Electro Analytical and spectrophotometric methods. 18 h


Flame emission and atomic absorption spectrometry. Instrumentation for AAS. The flame characteristics. Atomiser used in spectroscopy. Hollow cathode lamp. Interference in AAS. Application of AAS.

References

10. A.W. Adamson,”Physical Chemistry of Surfaces”, Wiley India.
CA 234  Inorganic Chemistry Practicals -II  

Total-125 h

1. Estimation of simple mixture of ions (involving quantitative separation) by volumetric and Gravimetric methods.

2. Analysis of typical alloys and ores

3. Ion exchange separation of binary mixtures.

4. Spectral Interpretation of metal complexes using IR, UV-Vis. spectral data. Supplementary information like metal estimation, CHN analysis, conductivity measurements and magnetic measurements to be provided to the students. Assessment is based on arriving at the structure of the complex and assignment of IR spectral bands.

5. Interpretation of TG and DTA curves of metal oxalates/acetates/sulphates/chlorides in hydrated forms. Assessment is based on the identification of various stages.
References

4. Willard, Merrit and Dean, ‘Instrumental Methods of Analysis,’

CA 235 ORGANIC PRACTICALS-II

Total 125 h

A. Volumetric estimation of

1) Aniline  2) Phenol  3) glucose
4) Iodine value and saponification value of coconut oil


C. Spectral identification ( UV, IR, $^1$H NMR, $^{13}$C NMR, EI mass) of Organic compounds from a library of organic compounds

D. Separations of mixtures by Paper Chromatography

1) Separation of amino acids  2) Separation of dyes

E) Three stage preparation

1) Benzaldehyde → Benzoin (green synthesis with thiamine HCl) → benzil
133

benzilic acid

2) Phthalic acid → Phthalic anhydride → pthalimide → anthranilic acid

References

3. Vishnoi, Practical Organic Chemistry, Vikas
4. R.M Silverstein, Spectrometric identification of Organic compounds
5. F G Mann and BC saunders, Practical Organic Chemistry, Pearson
7. C.E Bella and DF Taber, Organic Chemistry laboratory, Thomson
8. Nelson Practical Biochemistry, wiley
10. P.D.L Lampman and Chriz, Introduction to organic Laboratory techniques, College publishing,
11. Monograph on green laboratory experiments, DST , Govt of India.
12. http://sdb.sriodb.aist.go.jp/sdb/cgi-bin/direct_frame_top.cgi

CA 236 PHYSICAL PRACTICALS –II Total 125 h

1. Conductometry

Determination of strength of strong and weak acids in a mixture
Determination of strength of a weak acid.
Determination of solubility product of a sparingly soluble salt (PbSO₄, BaSO₄ etc.)
Hydrolysis of NH₄Cl or CH₃COONa or aniline hydrochloride
Determination of order of reaction, rate constant and energy of activation for saponification of ethyl acetate
Precipitation titrations.
Determination of critical micellar concentration (CMC) of sodium lauryl sulphate from measurement of conductivities at different concentrations.
Equivalent conductance at infinite dilutions and verification of Kohlraush’s Law.
Determination of Onsager constants.

2. Potentiometry
Determination of emf of Daniel cell.
Determination of the emf of various \( \text{ZnSO}_4 \) solutions and hence the concentration of unknown \( \text{ZnSO}_4 \) solution.
Determination of valency of mercurous ion.
Determination of temperature dependence of EMF of a cell
Determination of stoichiometry and formation constant of silver-ammonia complex.
Determination of activity and activity constant of electrolytes.
Determination of thermodynamic constants of reactions.
pH metric titrations.
Acid alkali titrations using Quinhydrone electrode.
Titrations(double) involving redox reactions – \( \text{Fe}^{2+} \) Vs \( \text{KMnO}_4 \), \( \text{K}_2\text{Cr}_2\text{O}_7 \), \( \text{Ce(NH}_3\text{)}_4\text{SO}_4 \) and \( \text{KI} \) Vs \( \text{KMnO}_4 \)
Determination of strengths of halides in a mixture.
Determination of pH of buffer solutions and hence to calculate the \( E_0 \) of quinhydrone electrode

3. Spectrophotometry
Verification of Beer-Lambert’s law.
Absorption spectra of conjugated dyes.
Determination of concentration of potassium dichromate and potassium permanganate in a mixture.
To study the complex formation between \( \text{Fe}^{3+} \) and salicylic acid.
Determination of pKa of an indicator.

4. Polarimetry
Measurement specific rotation of glucose.
Determination of specific rotation of sucrose
Determination of unknown concentration of glucose solution.
and rate constant of its hydrolysis in presence of HCl

5. Polarography :
Determination of half wave potential \( E \ ½ \) and unknown concentration of \( \text{Cd}^{2+} \) ion.
Determination of concentrations of metal ions in a mixture.

6. Surface tension
Determination of surface tension of various liquids by Stalagmometric method (drop number / drop weight)
Determination of parachors of molecules and various groups.
Determination of concentration of a mixture.
Determination of surface tension and paracho of liquids using double capillary method.

7. Refractometry
Determination of molar refraction of pure liquids
Determination of concentration of KCl solution/glycerol solution
Determination of solubility of KCl in water.
Determination of molar refraction of solid KCl
Study the stoichiometry of potassium iodide-mercuric iodide complex.
Determination of concentration of KI solution.

8. Viscosity
Determination of viscosity of various liquids using Ostwald’s viscometer.
Determination of unknown composition of given liquid mixture like toluene-nitrobenzene.
Verification of Kendall’s relation.
Verification of Jon Dole’s equation.

References
A.M.James, and F.E.Pichard, “Practical Physical Chemistry”, Longman.
B.Viswanathan, “Practical Physical Chemistry”, Viva Publications.
SEMESTER IV

CA 241 APPLIED CHEMISTRY

UNIT I  Water treatment

Boiler Troubles: Carry Over, Priming, Foaming, Scale, Sludge, Corrosion, Caustic Embrittlement.
Internal treatment of water: Carbonate conditioning, Phosphate conditioning, Colloidal conditioning, Calgon conditioning.

UNIT II  Petroleum, fuels & combustion, lubricants

Fuels & Combustion: Classification, Calorific value, Types, Determination by Bomb calorimeter, Dulong's Formula, Analysis of Coal, Proximate and Ultimate analysis, Fuel gas analysis, Significance, Numericals, Carbonization of Coal, Manufacture of metallurgical coke by Otto Hoffman's byproduct oven, Combustion calculations.
Lubricants: Functions of lubricant, Mechanism of lubrication, Fluid or Hydrodynamic Lubrication, Thin film or Boundary lubrication & Extreme pressure lubrication. Lubricants for Extreme ambient conditions and for special applications. Properties of lubricants and tests.
UNIT III  Corrosion and protective coatings


Protective coatings: Paints: Constituents, functions & mechanism of drying. Varnishes and Lacquers; surface preparation for metallic coatings, electroplating (gold) and electrodeless plating (Nickel), anodizing, phosphate coating, powder coating & antifouling coating.

UNIT IV  Applied inorganic chemistry

18 h


Refractories: Definition, Classification with Examples; Criteria of a Good Refractory Material; Causes for the failure of a Refractory Material. Flow sheet and engineering aspect of the manufacture of Refractories.

UNIT V  Applied organic chemistry

Raw materials and routes to major organic products. Flow sheets and engineering aspects of the manufacture of important products such as nitrobenzene, vinyl chloride, soaps, detergents and hydrogenation of oils.

Pharmaceuticals: manufacturing process of aspirin, vitamin A and paracetamol.

Cosmetics: Talcum Powder, Tooth pastes, Shampoos, Nail Polish, Perfumes, soaps, and detergents - General formulations and preparation - possible hazards of cosmetics use.

Adulterants: Adulterants in milk, ghee, oil, coffee powder, tea, asafoetida, chilli powder, pulses and turmeric powder - identification. Colour chemicals used in food-soft drinks and its health hazards


References

5) Environmental Chemistry-Collin Baird, Publisher WH Freeman, 2008
8) Environmental Chemistry - A .K. DE
9) Industrial Chemistry, B.K. Sharma- Goel publishing house, Meerut.
13) Applied Chemistry - K.Bagavathi Sundari - MJP Publishers
CA 242 DISSERTATION

Each of the students has to carry out original research in a topic in accordance with the Elective paper chosen for Semester IV under the guidance and supervision of a teacher in the concerned Department of the College.

Instructions to Question Papers Setters

The Syllabus of each theory has five units. While setting the question papers, equal weight is to be given to each of the Units for choosing the questions. Each question paper is of 3 hours duration and has three Sections, namely Section A, Section B and Section C constituting a total 75 marks as detailed.

Section A- Five questions, one from each Unit containing three short answer questions marked (a), (b), and (c), each of which has 2 marks. One has to answer any two of (a), (b) or (c) from each of the five questions. (2x10 = 20 marks)

Section B- Five questions, one from each Unit containing two short essay questions marked (a) and (b), each of which has 5 marks. One has to answer either (a) or (b) from each of the five questions. (5x5 = 25 marks)

Section C- Five essay questions, one from each unit having 10 marks. One has to answer any three questions from the five questions asked.(10x3 = 30 marks)