UNIVERSITY OF MYSORE

MODIFIED SYLLABUS FOR M. Sc. DEGREE COURSE
(CHOICE BASED-SYSTEM-SEMESTER SCHEME)

CHEMISTRY

2007-2008

SCHEME OF EXAMINATION UNDER THE SEMESTER SYSTEM

SCHEME OF STUDY AND EXAMINATION

FIRST SEMESTER

I. TUITION WORK

Course No.	Subject	Contact Hrs/Week	Credits per week	Examination Hours
(i)	**Theory**			
CH 101	Fundamentals of chemical analysis	3	3	2.5
CH 102	Modern concepts in inorganic chemistry	3	3	2.5
CH 103	Organic reaction mechanisms	3	3	2.5
CH 104	Quantum chemistry and nuclear chemistry	3	3	2.5
CH 105	Electrochemistry and computers for chemists	3	3	2.5
CH 106	Molecular symmetry and stereochemistry	3	3	2.5
(ii)	**Practicals**			
	Analytical/Inorganic practicals (50% of students)	8	2/2	6
	Organic/Physical practicals (50% of students)	8	2/2	6

II. SCHEME OF EXAMINATION

	Max. Marks
(i) Theory:	50 / Paper **50 x 6 = 300 Marks**
(ii) Practicals:	50 / Subject **50 x 2 =100 Marks**
(iii) Internal assessment	
Theory Test (all papers)	10 x 6 = 60 Marks
Home assignment (all papers)	5 x 6 = 30 Marks
Practicals	5 x 2 = 10 marks
	100 Marks

Total marks for I Semester **:** **500 Marks**

SECOND SEMESTER

I. TUITION WORK

Course No.	Subject	Contact Hrs/Week	Credits per week	Examination Hours
(i)	**Theory**			
CH 201	Separation techniques	3	3	2.5
CH 202	Co-ordination chemistry	3	3	2.5
CH 203	Synthetic organic chemistry	3	3	2.5
CH 204	Thermodynamics and statistical mechanics	3	3	2.5
CH 205	Chemical spectroscopy – I	3	3	2.5
CH 206	Photochemistry and radiation chemistry	3	3	2.5
(ii)	**Practicals**			
	Analytical/Inorganic practicals (50% of students)	8	2/2	6
	Organic/Physical practicals (50% of students)	8	2/2	6

II. SCHEME OF EXAMINATION

	Max. Marks
(i) Theory:	50 / Paper **50 x 6 = 300 Marks**
(ii) Practicals:	50 / Subject **50 x 2 =100 Marks**
(iii) Internal Assessment	
Theory Test (all papers)	10 x 6 = 60 Marks
Home assignment (all papers)	5 x 6 = 30 Marks
Practicals	5 x 2 = 10 marks
	100 Marks

Total marks for II Semester **:** **500 Marks**

THIRD SEMESTER

I. TUITION WORK

Course No.	Subject	Contact Hrs/Week	Credits per week	Examination Hours
(i)	**Theory**			
CH 301	Electroanalytical, optical and thermal methods of analysis	3	3	2.5
CH 302	Organometallic chemistry	3	3	2.5
CH 303	Heterocyclic chemistry, molecular rearrangement and synthetic drugs	3	3	2.5
CH 304	Chemical kinetics	3	3	2.5
CH 305	Chemical spectroscopy – II	3	3	2.5
CH CBCBS-1	General chemistry	4	4	3.0
(ii)	**Practicals**			
	Analytical/Inorganic practicals (50% of students)	8	2/2	6
	Organic/Physical practicals (50% of students)	8	2/2	6

II. SCHEME OF EXAMINATION

	Max. Marks
(i) Theory:	50 / Paper **50 x 4= 200 Marks**
(ii) Practicals:	50 / Subject **50 x 2 =100 Marks**
(iii) Internal Assessment	
Theory Test(all papers)	10 x 4 = 40 Marks
Home assignment (all papers)	5 x 4 = 20 Marks
Practicals	5 x 2 = 10 Marks
Seminar	30 Marks
	100 Marks
(iv) For CH CBCBS-1:	
Theory	80 Marks
Internal Assessment	
Theory test + Home Assignment	10 + 10 = 20 Marks

Total marks for III Semester **: 500 Marks**

FOURTH SEMESTER

I. TUITION WORK

Course No.	Subject	Contact Hrs/Week	Credits per week	Examination Hours
	(i) Theory			
CH 401	Bioanalytical chemistry	3	3	2.5
CH 402	Bioinorganic chemistry	3	3	2.5
CH 403	Bioorganic chemistry	3	3	2.5
CH 404	Biophysical chemistry	3	3	2.5
CH 405	Dissertation / Project	3	3	-
CH 406	**Elective papers**			
	(i) Chemical Biology	3	3	2.5
	(ii) Chemistry in industry			
	(iii) Environmental Chemistry			
	(iv) Natural products			
	(v) Pharmacokinetics			
	(vi) Polymer chemistry			
	(vii) Solid state chemistry			
	(ii) Practicals			
	Analytical/Inorganic practicals (50% of students)	8	2/2	6
	Organic/Physical practicals (50% of students)	8	2/2	6

II. SCHEME OF EXAMINATION

	Max. Marks
(i) Theory:	50 / Paper **50 x 6 = 300 Marks**
(ii) Practicals:	50 / Subject **50 x 2 =100 Marks**
(iii) Internal Assessment	
Theory (**all papers except dissertation**)	10 x 5 = 50 Marks
Practicals	10 x 2 = 20 Marks
Seminar	30 marks
	100 Marks

Total marks for IV Semester	**500 Marks**
Grand total for all the Semesters	**2000 Marks**

GENERAL REQUIREMENTS

(i) MINIMUM FOR PASS

There will be minimum of 40 percent in each theory paper and practicals and 50% in aggregate including internal assessment marks. However, there is no minimum marks for internal assessment.

(ii) CARRY OVER

The candidate is permitted to attend the course (all the four semesters) irrespective of the results in each semester.

(iii) CLASS DECLARATION

The marks secured by the candidate in his/her first appearance shall be taken for class declaration at the end of fourth semester.

(iv) SYLLABUS

Each theory paper in the semester system shall have 48 contact hours instructions.
Each practical paper in the semester system shall have 120 contact hours and 30 min for seminar for each candidate.
The dissertation work in the Semester System shall have 120 working hours and 30 minutes for Seminar, for each candidate. Every candidate has to submit a dissertation at the end of the semester for evaluation and viva-voce examination.

(v) EXEMPTION

As per the existing University Rules of Semester System

(vi) QUESTION PAPERS

Each theory paper in semester system shall consist of one compulsory short answer type questions of TEN marks (Ten questions of one mark each) and SIX questions of TEN marks each of which a candidate has to answer FOUR. Each question consists of sub-divisions (a), (b) and (c).
The examiner shall set the question paper evenly distributed amongst entire syllabus.
Two experiments (one from each part) are to be set for each practical examination and each experiment carries 25 marks.

(vii) INTERNAL ASSESSMENT

(a) There shall be one theory test in the middle of each semester.
(b) There shall be continuous assessment of the candidates in the practicals including practical records till the end of the semester and the average marks secured by the candidate for a maximum of 5 marks shall be taken.

(viii) IMPROVEMENT

As per the existing University Rules of Semester system.

(ix) 'General Chemistry' paper in the third semester - CH-CBCBS-I is a 'choice based – Credit based System' paper introduced to accommodate students from other Departments. The students of Chemistry Department have to take any four out of the five available papers (for 200 marks) in addition to the 'Choice based - Credit based System' paper offered by any one of the other Departments (for 100 marks), in the third semester.

(x) CH 406

This is an elective paper and the students have option to select any one of the seven papers under CH 406. But the minimum number of students for any of the papers under **CH 406** is **TEN.** If the required number of students are less than the minimum number, then the students shall opt for other papers in CH 406 where ever the number of candidates exceeds **TEN.**

(xi) Credits

There shall be three credits/week per theory paper and two credits/week per practical paper. i.e., one contact hour in theory per paper is equivalent to ONE CREDIT and four contact hours in practical per paper is equivalent to ONE CREDIT. In the case of CH CBCBS-1, four credits per week is offered.

FIRST SEMESTER

CH 101 – FUNDAMENTALS OF CHEMICAL ANALYSIS

(48 HOURS)

UNIT-I

Statistical Treatment of Analytical Data and Sampling: Limitations of analytical methods. Classification of errors-systematic errors-sources, effects and their reduction. Random errors-sources and distribution. Accuracy and precision. Measures of central tendency and variability. Reliability of results-confidence interval. Comparision of results-Student's t-test, comparing the two means and standard deviations-F-test, t-test and paired t-test. Rejection of a result-Q-test. Number of replicate determinations. Control charts. Correlation and regression-correlation coefficient, linear regression, errors in slope and intercept, error in the estimate of concentration. Detection limits, Sampling and sample handling-representative sample, sample storage, sample pretreatment and sample preparation. Hazards in sampling. Quality in analytical laboratories-quality control and quality assurance, accreditation system. **[16 HOURS]**

UNIT-II

Gravimetric analysis: General principles, stoichiometry, calculation of results from gravimetric data. Properties of precipitates. Nucleation and crystal growth, factors influencing completion of precipitation. Co-precipitation and post-precipitation, purification and washing of precipitates. Precipitation from homogeneous solution, a few common gravimetric determinations-chloride as silver chloride, sulphate as barium sulphate, aluminum as the oxinate and nickel as dimethyl glyoximate.
Acid base titrations: Principles of titrimetric analysis, titration curves for strong acid-strong base, weak acid-strong base and weak base-strong acid titrations, poly protic acids, poly equivalent bases, determining the equivalence point-theory of acid base indicators, colour change range of indicator, selection of proper indicator.
Applications of acid-base titrations: Determination of nitrogen, sulphur, ammonium salts, nitrates, and nitrites carbonates and bicarbonates, and organic functional groups like carboxylic acid, sulphonic acid, amine, ester, hydroxyl, carboxyl groups, air pollutants like SO_2.
Acid-base titrations in non-aqueous solvents: Role of solvent in Acid-base titrations, solvent systems, differentiating ability of a solvent, some selected solvents, titrants and standards, titration curves, effect of water, determining the equivalence point, typical applications-determination of carboxylic acids, phenols and amines. **[16 HOURS]**

UNIT-III

Precipitation titrations: Titration curves, feasibility of precipitation titrations, factors affecting shape-titrant and analyte concentration, completeness of the reaction, titrants and standards, indicators for precipitation titrations involving silver nitrate the Volhard, the Mohr and the Fajan's methods, typical applications.
Complexometric titrations: Complex formation reactions, stability of complexes, stepwise formation constants, chelating agents, EDTA-acidic properties, complexes with metal ions, equilibrium calculations involving EDTA, conditional formation constants, derivation of EDTA titration curves, effect of other complexing agents, factors affecting the shape of titration curves-completeness of reaction, indicators for EDTA titrations-theory of common indicators, titration methods employing EDTA-direct, back and displacement titrations, indirect determinations, titration of mixtures,

selectivity, masking and demasking agents, typical applications of EDTA titrations-hardness of water, magnesium and aluminium in antacids, magnesium, manganese and zinc in a mixture, titrations involving unidentate ligands-titration of chloride with Hg^{2+} and cyanide with Ag^{+}. **[16 HOURS]**

REFERENCES

1. Fundamental of Analytical Chemistry, D.A. Skoog, D.M. West, Holler and Crouch 8th edition, 2005, Saunders College Publishing, New York.
2. Analytical Chemistry, G.D. Christian, 5th ed., 2001 John Wiley & Sons, Inc, India.
3. Quantitative Analysis, R.A. Day and A.L. Underwood, 6th edition,1993 prentice Hall, Inc. New Delhi.
4. Vogel's Textbook of Quantitative Chemical Analysis, J. Mendham, R.C. Denney, J.D. Barnes and M.J.K. Thomas, 6th edition, Third Indian Reprint.2003 Pearson Education Pvt. Ltd., New Delhi.
5. Analytical Chemistry Principles, John H. Kennedy, 2nd edition, Saunders College Publishing, California, 1990.

CH. 102 – MODERN CONCEPTS IN INORGANIC CHEMISTRY

[48 HOURS]

UNIT –I

Ionic Bond: Properties of ionic substances, structures of crystal lattices (Nacl, CsCl, ZnS, Wurtzite and rutile). Lattice energy, Born-Haber cycle, uses of Born-Haber type calculations, Born-Lande equation. Ionic radii, factors affecting the radii of ions, radius ratio effects, covalent character in ionic bonds, hydration energy and solubility of ionic compounds.

Covalent Bond: M.O. treatment for homonuclear and heteronuclear diatomic molecules. M.O. treatment involving delocalized πbonding (CO_3^{2-}, NO_3^-, NO_2^-, CO_2 and N_3^-). Weak interactions in covalent substances. VSEPR model for explaining structure of molecules including fluxional molecules, short comings of the VSEPR model. **16 HOURS]**

UNIT –II

Modern concepts of acids and bases: Lux-Flood and Usanovich concepts, solvent system and leveling effect. Hard –Soft Acids and Bases Classification and Theoretical backgrounds.

Non-aqueous solvents: Classification of solvents**,** Properties of solvents (dielectric constant; donor and acceptor properties) protic solvents (anhydrous H_2SO_4, HF and glacial acetic acid), aprotic solvents (liquid SO_2 and N_2O_4). Solutions of metals in liquid ammonia, hydrated electron, complex hydrides of boron and aluminium, halogens in positive oxidation states, astatine and psuedo halogens.

[16 HOURS]

UNIT –III

Correlation of general properties of d-block elements with those of 4f and 5f elements.

Lanthanide series: Introduction, electronic structure, oxidation states, lanthanide contraction, abundance and extraction, lanthanides as shift reagents.

Separation of lanthanides: Solvent extraction and ion-exchange. Chemical properties of compounds of lanthanides in II, III, and IV oxidation states. Magnetic properties, colour and spectra.

Actinides: Electronic structure and position in the periodic table, oxidation states, occurrence and synthesis of the elements. Spectral and magnetic properties of compounds of actinides in comparison with those of lanthanides and d-block elements.
Uranium: Isotope separation/enrichment, Chemical properties, hydrides, oxides and halides. Chemistry of trans-uranium elements. **[16 HOURS]**

REFERENCES

1. Inorganic Chemistry (4^{th} edition): J.E. Huheey, E.A. Keiter and R.L. Keiter (1993); Harper Collins.
2. Introduction to modern inorganic chemistry (4^{th} edition): K.M. Mackay and R.A. Mackay (1989): Blackie.
3. Advanced Inorganic Chemistry (5^{th} edition): F.A. Cotton and G. Wilkinson (1990): Wiley.
4. Concise Inorganic Chemistry (5^{th} edition): J.D. Lee (2000); Blackwell Science.
5. Concepts and Models of Inorganic Chemistry (3^{rd} edition): B.E. Douglas, D.H. Mc Daniel and Alexander. (2001): Wiley.
6. Chemistry of the Elements: Greenwood and Earnshaw. (1986): Pergamon Press.
7. Inorganic Chemistry (3^{rd} edition): Shriver, Atkins and Langford (1999); Oxford Univ. Press.

CH 103 – ORGANIC REACTION MECHANISMS

[48 HOURS]

UNIT-I

Structure and reactivity: Acids and Bases, Structural effects on acidity and basicity, hydrogen bonding, resonance, inductive and hyperconjugation effects.
Reaction intermediates: Formation, structure, stability, detection and reactions of carbocations (classical and non-classical), carbanions, free radicals, carbenes, nitrenes, nitrile oxides, nitrile imines, nitrile ylides and arynes.
Enamines: Formation and reactions, Stork-enamine reactions.
Ylides: Nitrogen, sulphur and phosphorous ylides.
Umpoulong synthesis: Acyl anion equivalents and their application in organic synthesis.

[16 HOURS]

UNIT-II

Reaction Mechanism I: Clasification of reactions, meaning and importance of reaction mechanism.
Determination of reaction mechanism by kinetic and non-kinetic methods:
Kinetic method: Mechanistic implications from rate laws, the transition state theory, ambiguities in interpreting kinetic data, solvent effect, ionic effect, isotopic effect, solvent isotopic effect, substituent effect, steric effect, linear free energy relationships – Hammett equation and Taft treatment.**Non-kinetic methods**: Energy profile diagram, identification of products, testing possible intermediates, trapping of intermediates, cross over experiments, isotopic labeling, sterochemical studies, limitations of reactions.
Substitution reactions: Mechanism of nucleophilic substitution reactions – Kinetics, mechanism and stereochemical factor affecting the rate of S_N^1, S_N^2, S_{RN}^i, S_N^i, $S_N^{1'}$, $S_N^{2'}$, S_N^{1i}, reactions, Neighbouring group participation.

Mechanism of electrophilic substitution reactions – Kinetics, mechanism and stereochemical factor affecting the rate of S_E1 & S_E2

Elimination reactions:Mechanism and stereochemistry of eliminations –E1, E2, E1cb mechanism, cis elimination, Hofmann and Saytzeff eliminations, competition between elimination and substitution, Chugaev reaction. **[16 HOURS]**

UNIT-III

Reaction Mechanism II: Mechanism of Addition reactions: Addition to C-C multiple bonds involving electrophiles, nucleophiles and free radicals. Markownikoff's rule and anti-Markownikoff's rule, Hydroboration and its application.

Typical additions to carbonyl compounds: Addition of hydride, water, alcohol, thioalcohol, bisulphite, HCN, Grignard reagents and amino compounds.

Mechanism of reactions of carboxylic acids and their derivatives: Mechanism of ester hydrolysis formation, formation and hydrolysis of amides, decarboxylation mechanisms.

Aromatic electrophilic substitution: Mechanism of nitration, halogenation, sulphonation, Friedel-Crafts alkylation and acylation, Mannich reaction, chloromethylation, Vilsmeier-Haack reaction,

Aromatic nucleophilic substitution: S_N^1, S_N^2 and benzyne mechanism, Bucherer reaction.

[16 HOURS]

REFERENCES

1. H. Pine, Hendrickson, Cram and Hammond, Organic Chemistry, Mac Grow Hill, New York, 1987.
2. Organic Chemistry – Morrison & Boyd
3. I. Finar, Organic Chemistry, ELBS Longmann, Vol. I & II,
4. 1984
5. Basic Principles of Organic Chemistry – Robert & Casereo
6. N. S. Issacs, Reactive intermediates in Organic Chemistry, Jhon Willey and Sons, New York.1974.
7. R. K. Bansal, Organic Reaction Mechanism, Wiley Eastern Limited, New Delhi, 1993.
8. J. March, Advanced Organic Chemistry, Willey Interscience, 194.
9. E. S. Gould, Mechanism Mechanism and Structure in Organic Chemistry, Halt, Rinhart & Winston, New York, 964.
10. A Guide book to mechanism in Organic Chemistry – Petersyke
11. F. A. Carey and Sundberg, Advanced Organic Chemistry – Part A & B, 3rd edition, Plenum Press, New York, 1990.
12. S. K. Ghosh, Advanced General Organic Chemistry, Book and Alleied (P) Ltd, 1998.

CH 104 – QUANTUM CHEMISTRY AND NUCLEAR CHEMISTRY

[48 HOURS]

UNIT-I

Wave-particle duality of material particles, deBroglie equation, Heisenberg Uncertainty principle, Concept of operators (operator–operand), Algebra of operators, commutative and non-commutative operators, linear operator, Laplacian operator, Hamiltonian operator, eigen value, eigen function, class Q function, Hermitian operator, turn over rule, atomic units. Wave equation for stretched strings, Schrodinger wave equation for particles, Eigen values and Eigen functions, postulates of quantum mechanics. Application of Schrodinger equation to a free particle and to a particle trapped in a

potential field (one dimension and three dimensions). Degeneracy, Wave equation for H-atom, separation and solution of R, Φ and θ equations. Application of Schrodinger equation to rigid rotator and harmonic oscillator. **[16 HOURS]**

UNIT-II

Approximate methods –Necessity of approximate methods, perturbation method, the theory of perturbation method –first order and second order correction, application to He-atom (first order correction only) – calculation of first ionization potential and binding energy. Variation theorem-statement and proof. Application of variation theorem to a particle in one dimensional box, linear oscillator, H and He-atoms, SCF method for many electron atom. Slater Orbitals –Effective nuclear charge (ENC), expressions for slater orbitals for 1s, 2s, 3s, 2p and 3d electrons (no derivation), Slater's rules for calculation of ENC-Slater's orbitals for He, Carbon and nitrogen. Theories of valence – Introduction, linear and non-linear variation functions, secular equations, coulombic, exchange, normalization and overlap integrals, secular determinants. **[16 HOURS]**

UNIT-III

Nuclear chemistry: Radioactive decay – General characteristics, decay kinetics, parent –daughter decay growth relationships, determination of half-lives, Nuclear models –shell model, liquid drop model, Fermi gas model, Collective model and optical model, Nuclear stability –packing fraction, binding energy, proton –neutron ratio, magic number, nuclear stability with respect to beta decay. Theories of alpha, beta and gamma decays. Nuclear reactions –Bethe's notation, types of nuclear reactions –specific nuclear reactions, photonuclear reactions, fission and fusion reactions, Oppenheimer –Phillips process, spallation reactions, conservation in nuclear reactions, reaction cross section.

Definition of curie and related calculations, preparation of artificial radionuclides by bombardment radiochemical separation techniques (carriers, solvent extraction and ion exchange), Szilard-Chalmers process.

Experimental techniques in the assay of radioisotopes, gas filled detectors-ionization chamber, proportional and Geiger-Muller counters –G.M. Plateau, dead time, coincidence loss, determination of dead time, scintillation counters, solid state detectors. **[16 HOURS]**

REFERENCES

1. Quantum Chemistry – A.K. Chandra. Second Edition, Tata McGraw Hill Publishing Co. Ltd., (1983).
2. Quantum Chemistry – Eyring, Walter and Kimball. John Wiley and Sons, Inc., New York.
3. Quantum Chemistry –I.N. Levine. Pearson Education, New Delhi, (2000).
4 Theoretical Chemistry – S. Glasstone. East West Press, New Delhi, (1973).
5. Quantum Chemistry – R.K. Prasad, New Age International Publishers, (1996).
6. Valence Theory – Tedder, Murel and Kettle.
7. Quantum Chemistry – D.A. McQuarrie.
8. Theoretical Inorganic Chemistry – Day and Selbin
9. Nuclear Chemistry by Friedlander and Kennedy, John Wiley and Sons (1987).
10. Nuclear Physics and Chemistry by G. Harvey.
11. Essentials of Nuclear Chemistry by H.J. Arnikar, Eastern Wiley (1990).
12. Nuclear Chemistry by U.N. Dash, Sultan Chand and Sons (1991).
13. Source book on atomic energy by S. Glasstone, 3rd edition Van Nonstrand (1967).

14. Nuclear chemistry by Friedlander and Kennedy, John Wiley and Sons (1987).
15. Essentials of nuclear chemistry by H.J. Arnikar, Eastern Wiley (1990).
16. Source book on atomic energy by S. Glasstone, 3rd edition, Van No strand (1967).
17. Nuclear radiation detection by Price. Nuclear radiation detectors by S.S. Kapoor and Ramamoorthy, Wiley Eastern (1986).
18. Fundamentals of radiochemistry by D.D. Sood, A.V.R. Reddy and N. Ramamoorthy, Indian Association of Nuclear Chemists and Allied Scientists, 2nd edition (2004).

CH 105 – ELECTROCHEMISTRY AND COMPUTERS FOR CHEMISTS

[48 HOURS]

UNIT-I

Arrhenius theory of strong and weak electrolytes and its limitations, Debye-Huckel theory of strong electrolytes, Debye Huckel-Onsager equation, Debye-Huckel limiting equation for activity coefficients, Debye-Huckel equation for appreciable concentrations. A brief survey of Helmholtz-Perrin, Gouy-Chapman and Stern electrical double layer. Liquid junction potential and its determination. Transport Number**:** Determination of transport number by Hittorf method and e.m.f method. True and apparent transport numbers. Abnormal transport numbers, effect of temperature and concentration on transport number. Energetics of cell reactions, effect of temperature, pressure and concentration on energetics of cell reactions (calculation of ΔG, ΔH and ΔS). Electrochemical energy sources –Batteries, classification, characteristics, primary, secondary and lithium batteries.

[16 HOURS]

UNIT-II

Irrversible electrode process: Introduction, reversible and irreversible electrodes reversible and irreversible cells. Polarization, over voltage-ohmic over voltage, concentration overvoltage activation overvoltage, experimental determination of over voltage. Equations for concentration over potential, diffusion current –stationary current, potential curves, thickness of diffusion layer, diffusion controlled current –potential curves at a dropping mercury electrode, polarography, half wave potential, application in qualitative and quantitative analysis. Energy barrier and electrode kinetics, Butler-Volmer equation, Tafel equation. Hydrogen over voltage-mechanism, bubble formation theory, Tafel's theory, Gurney's quantum mechanical theory. Eyring- Laidler-Glasstone theory, Oxygen over voltage. Effect of temperature, current density and pH on over voltage.
Corrosion: Manifestations of corrosion, types of corrosion, basis of electrochemical corrosion, theories of corrosion. Local cell theory (Wagner and Traud theory) Current –potential relations (Evan diagram) in corrosion cells. Effect of pH, nature of metal and dissolved oxygen (principle of differential aeration) on corrosion. Corrosion inhibition and prevention by painting, phosphating, corrosion protection by Anodic (passivation) and cathodic protection. **[16 HOURS]**

UNIT – III

Computers: Introduction to computers and computing: Basic Structure and functioning of computers with a PC as an illustrative example. I / O devices, Memory, Secondary Storage, Computer languages, Operating Systems, Introduction to Windows, Introduction to Algorithms and Flow-charts.

Basic: Elements, principles of Basic programming, GW Basic and visual Basic, chemistry and Basic programming.

Fortran: Principles of Fortran programming, chemistry and Fortran programming. A very brief account of C-programming and chemistry applications.

Computer Programming in C: C Fundamentals, the characters set, Identifiers and key words, data types - constants and variables, declarations, expressions and operators. Data Input and Output. Control Statements, Functions and Arrays.

Application of C-language in Chemistry: Development of small computer codes for solving simple formulae in chemistry such as Van der waals' Equation, pH titration, Kinetics of radioactive decay, Evaluation of lattice energy and ionic radii from experimental data, Linear and simultaneous equations to solve secular equations within the Huckel Theory.

Applications of computers in chemistry: (including practical demonstrations),

Programming examples (using basic, Fortran, spreadsheet and 'C') to handle the following numerical methods in chemistry-least square fit, solution of simultaneous equation, polynomial equation, graphic kinetics (Montecarlo simulations of kinetics), potentiometric titrations and end point location. Fitting curves and plotting functions. Simulation studies, elements of molecular modeling.

[16 HOURS]

REFERENCES

Electrochemistry

1. Elements of Physical Chemistry –Lewis and Glasstone.
2. Physical Chemistry by P.W. Atkins, ELBS, 4th Edition, Oxford University Press (1990).
3. Introduction to electrochemistry by S. Glasstone
4. Modern electrochemistry Vol. I and II, by J.O.M. Bockris and A.K.N. Reddy, Plenum Press, New York (1970).
5. Chemical and Electrochemical energy systems, by R. Narayan and B. Viswanathan, Universities Press (India) (1998).
6. Electrochemistry –Principles and applications by E.G. Potter.
7. Electrochemistry by Reiger, Prentice Hall (1987).
8. Treatise on Electrochemistry, G. Kortum 2nd Edition, Elsevier, London (1965).
9. Electrochemisty, Principles and Application: E.G. Potter.
10. Basic Physical Chemistry by W.J. Moore, Prentice Hall, New Delhi, (1986).
11. Physical Chemistry –G.M. Barrow, McGraw Hill International service (1988).

Computers:

12. R.Hunt and J.Shelly: Computer and Common Sense (Prentice Hall)
13. V.Raja Raman and T.Radhakrishna: An Introduction to Digital Computer Design (Prentice Hall)
14. A.C.Norris: Computational Chemistry
15. J.P.Killngbeck and Adam Hilger: Microcomputer Quantum Mechanics
16. E.Balaguruswamy: Programming in 'ANSI C ' , Second Ed. (Tata McGraw Hill)
17. Theory and Problems of Computing with Basic, B.G. Gottfried, Mc Graw Hill, New York.
18. Quantitative Analysis, R.A. Day and A.L. Underwood, 6th edition, prentice Hall, Inc. 1999.
19. Computer Programming in Fortran IV, V. Rajaraman, -Prentice Hall, India
20. Fortran IV for Computers, P.N. Arora and H. Singh, S. Chand and Co., New Delhi.
21. C Programming Principles and Practices, M.T. Gardy, Mc Graw Hill.
22. Illustrated C Programming, J. E. Bean, B.P.B. Publications, Delhi.

CH 106 – MOLECULAR SYMMETRY AND STEREO CHEMISTRY

[48 HOURS]

UNIT-I

Molecular symmetry: Symmetry elements and symmetry operations, rotation axis, rules for orientation of molecules, plane of symmetry, rotation-reflection axis, centre of symmetry and identity element of symmetry. Correlation of Schoenflies and Hermann-Maugin Symbols for symmetry elements. Products of symmetry operations. General relations among symmetry elements and symmetry operations.

Group theory: Concept of a group, definition of a point group, procedure for classification of molecules into point groups. Schoenflies and Hermann-Maugin symbols for point groups. Properties and definitions of group theory. Multiplication tables for the symmetry operations of simple molecules. International (Hermann-Maguin) notations, subgroups. Matrix notation for the symmetry elements and for geometric transformations. Class of a group and similarity transformation.

[16 HOURS]

UNIT-II

Representation of groups: Reducible and irreducible representations. The Great Orthogonality theorem and its consequences. Character tables (C_s, C_i, C_2, C_{2v}, C_{2h} and C_{3v}). Labelling of irreducible representations. Group theory and hybrid orbitals to form bonds.

Applications of group theory: Applications of group theory to crystal field theory. Bonding in octahedral and tetrahedral complexes. Symmetry and dipole moments, symmetry and optical activity.

Molecular vibrations: Introduction, symmetry of normal vibrations, determining the symmetry types of normal modes, selection rules for fundamental vibration transitions.

Representation of vibrational modes in non-linear molecules. Group theory and linear molecules (Integration method). Vibrations in polyatomic molecules. **[16 HOURS]**

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UNIT-III

Stereoisomerism: Projection formulae [Fly wedge, Fischer, Newman and Saw horse], enantiomers, diasteroisomers, racemic mixture and their resolution, configurational notations of simple molecules, DL and RS configurational notations.

Stereoselectivity: Stereoselective reactions, diasteroselective reactions, stereospecific reactions, regioselective & regiospecific reactions.

Optical isomerism: Conditions for optical isomerism, optical isomerism due to chiral centers and molecular dissymmetry, allenes and biphenyls, criteria for optical purity.

Geometrical isomerism: Due to C=C, C=N and N=N bonds, E,Z conventions, determination of configuration by physical and chemical methods.

Conformational isomerism: Elementary account of conformational equilibria of ethane, butane and cyclohexane.

Conformational analysis: Conformation of cyclic compounds such as cyclopentane, cyclohexane, cyclohexanone derivatives and decalins. Conformational analysis of 1,2-; 1,3-, 1,4-disubstituted cyclohexane derivatives and D-Glucose. Effect of conformation on the course of rate of reactions.

[16 HOURS]

REFERENCES

1. E. L. Eliel and S. H. Wilen, Stereochemistry of Organic Compounds, Jhon Willey and Sons, New York. 1994.

2. Introduction to stereochemistry – K. Mislow.
3. Stereochemistry and mechanism through solved problems – P. S. Kalsi
4. D. Nasipuri, Stereochemistry of Organic Compounds, 2nd edition, Wiley Eastern Limited, New Delhi, 1991.
5. Symmetry in Chemistry, - H. Jaffe and M. Orchin, John Wiles, New York, (1965).
6. Symmetry in Molecules, - J.M. Hollas, Chapman & Hall Ltd., London, (1972).
7. Chemical Applications of Group Theory, - F.A. Cotton, Wiley Eastern Ltd., 2nd Edition, New Delhi, (1971).
8. Group theory and Symmetry in Chemistry, -G. Raj, A. Bhagi and V. Jain, Krishna Prakashan Media (P) Ltd., Meerut, (1998).
9. The determination of Molecular Structure–P.J. Wheatley, Oxford University Press, Oxford, (1969).

FIRST SEMESTER PRACTICALS

ANALYTICAL CHEMISTRY PRACTICALS

[120 HOURS]

PART-I

1. Determination of carbonate and bicarbonate in a mixture by pH-metric titration and comparision with visual acid-base titration.

2. Determination of total acidity of vinegar and wines by acid-base titration.

3. Determination of aniline by non-aqueous acid-base titration.

4. Determination of total hardness of water by complexation titration using EDTA.

5. Determination of percentage of chloride in a sample by precipitation titration-Mohrs, Volhard and Fajans methods.

6. Determination of copper in an ore/ an alloy by iodometric redox titration.

7. Determination of ascorbic acid in vitamin C tablets by titrations with $KBrO_3$.

8. Determination of vitamin C in citrus fruit juice by iodimetric titration.

9. Potentiometric determination of the equivalent weight and Ka for a pure unknown weak acid.

10. Determination of iron in razor blade by visual and potentiometric titration using sodium metavanadate.

11. Determination of chloride content of an industrial effluent by conductometric titration with silver nitrate.

12. Photometric and potentiometric titrations of copper with EDTA.

13. Spectrophotometic determination of pH of an unknown buffer using a dye(Bromocresol green).

14. Determination of nitrate nitrogen in water by spectrophotometry using phenol disulphonic acid as chromogenic agent.
15. Spectrophotometric determination of creatinine in urine.
16. UV-spectrophotometric analysis of benzene in cyclohexane.
17. Gas chromatographic determination of ethanol in beverages.
18. Separation of metal ions by paper chromatography and their identification.
19. Thin-layer chromatographic separation of nitro anilines on fluorescent sheets.
20. Flame emission spectrometric determination of sodium and potassium in river/lake water.

PART-II

1. Determination of replaceable hydrogen and relative molecular mass of a weak organic acid by titration with NaOH.
2. Determination of total alkalinity of soda ash by visual and pH-metric titrations.
3. Determination of silver in an alloy by Volhard method.
4. Mercuricmetric determination of blood or urine chloride.
5. Analysis of commercial hypochlorite or peroxide solution by iodometric titration.
6. Determination of antimony in stibnite by titration with iodine.
7. Determination of sulphate in ground water by titration with $BaCl_2$ using an adsorption indicator.
8. Periodate determination of ethylene glycol(Malprade reaction).
9. Determination of calcium in milk powder by EDTA titration.
10. Determination of calcium in calcium gluconate/calcium carbonate tablets or injections by EDTA titration.
11. Determination of iron in pharmaceuticals by visual and potentiometric titration using cerium(IV) sulphate.
12. Determination of total cation concentration of tap water by ion-exchange chromatography.
13. Determination of magnesium in milk of magnesium tablets by ion-exchange chromatography.
14. Anion exchange chromatographic separation of zinc and magnesium followed by EDTA titration of the metals.
15. Electrolytic determination of copper in an ore/ an alloy.
16. Analysis of an industrial effluent for sulphate by conductometric titration with $BaCl_2$.
17. Spectrophotometric determination of manganese in steel.
18. Determination of iron as the 8-hydroxyquinolate by solvent extraction method.

19. Spectrophotometric determination of iron in natural water by thiocyante/orthophenanthroline method.

20. Spectrophotometric determination of molecular weight of a compound.

REFERENCES

1. Fundamental of Analytical Chemistry, D.A. Skoog, D.M. West, Holler and Crouch 8th edition, 2005, Saunders College Publishing, New York.
2. Analytical Chemistry, G.D. Christian, 5th ed., 2001 John Wiley & Sons, Inc, India.
3. Quantitative Analysis, R.A. Day and A.L. Underwood, 6th edition,1993 prentice Hall, Inc. New Delhi.
4. Vogel's Textbook of Quantitative Chemical Analysis, J. Mendham, R.C.
5. Denney, J.D. Barnes and M.J.K. Thomas, 6th edition, Third Indian Reprint.2003 Pearson
6. Education Pvt. Ltd., New Delhi.
7. Analytical Chemistry Principles, John H. Kennedy, 2nd edition, Saunders College Publishing, California, 1990.
8. Practical Clinical biochemistry methods and interpretations, R.Chawla, J.P. Bothers Medical Publishers (P) ltd., 1995.
9. Laboratory manual in biochemistry, J. Jayaraman, New Age International Publishers, New Delhi, 1981.
10. Practical clinical Biochemistry-Harold Varley and Arnold.Hein mann, 4th edn.
11. Environmental science: Laboratory Manual, Maurice A. Strabbe, The C.V.Mosbey Co. Saint Loucs, 1972.
12. Experiments on water pollution, D.I.Williams and D. Anglesia, Wayland Publishers Ltd, England, 1978.
13. Experiments on Land pollution D.I.Williams and D. Anglesia, Wayland Publishers Ltd, England, 1978.
14. Experiments in environmental chemistry,P.D.Vowler, and D.W.Counel, Pergamon press, Oxford 1980.
15. Manual soil Laboratory Testing-vol I, K.H. Head, Pentech Press, London 1980.

INORGANIC CHEMISTRY PRACTICALS

[120 HOURS]

PART–I

1. Analysis of Ores:

1. Hematite
    a. insoluble (gravimetrically)
    b. iron titrimetrically using cerium(IV) solution
2. Dolomite
    1. insoluble (gravimetrically)
    2. calcium and magnesium using EDTA
3. Pyrolusite
    1. insoluble (gravimetrically)
    2. Manganese dioxide titrimetrically using permanganate.

2. Micro-volumetric estimation of calcium using EDTA**.**

3. Analysis of alloys:

a) Solder – lead and tin using EDTA
b) Copper –nickel alloy
   (i) Copper volumetrically using KIO_3
   (ii) Nickel gravimetrically using DMG

4. Quantitative analysis of mixtures:

a) Chloride and iodide
   (i) iodide volumetrically using KIO_3
   (ii) total halide gravimetrically
b) Calcium and lead – using EDTA

5. Spectrophotometric determination of:

a) iron using thiocyanate/1,10-phenonthroline
b) chromium using diphenyl carbazide
c) nickel using dimethylglyoxime
d) titanium using hydrogen peroxide

6. Circular paper chromatography –separation of: (Demonstration)

a) iron and nickel
b) copper and nickel

PART–II

Semimicro qualitative analysis of mixtures containing TWO anions and TWO cations and ONE of the following less common cations.
W, Mo, Ce, Th, Ti, Zr, V, U and Li.

REFERENCES

1. A Text Book of Quantitative Inorganic Analysis – A.I. Vogel. III edition
2. Vogel's Text Book of Quantitative Chemical Analysis – J. Basset, R.C. Denney, G.H. Jeffery and J. Mendhom.
3. Spectrophotometric determination of elements – Z. Marczenko.
4. Vogel's Qualitative Inorganic Analysis – Svelha.
5. Macro and Semimicro inorganic qualitative analysis – A.I. Vogel.
6. Semimicro Qualitative Analysis – F. J. Welcher and R.B. Halin.

ORGANIC CHEMISTRY PRACTICALS

[120 HOURS]

PART-I

Organic Preparations: Preparations involving oxidation, reduction, dehydration, decarboxylation, halogenation, nitration, sulfonation, diazotization, cyclization, condensation, addition reactions.

1. Preparation of p-bromoaniline from acetanilide

2. Prpearation of p-nitroacetanilide from acetanilide
3. Prpearation of n-butyl bromide from n-butanol
4. Preparation of o-iodobenzoic acid from anthranilic acid
5. Preparation of aniline from nitrobenzene
6. Preparation of osazone derivative
7. Prpearation of penta-O-acetyl-D-glucose from glucose
8. Preparation of 3-methyl-1-phenyl-pyrazolone
9. Preparation of *cis* and *trans* cinnamic acid
10. Prearation of phenoxy acetic acid
11. Preparation of hippuric acid from glycine
12. Preparation of m-nitrobenoic acid from methyl benzoate
13. Preparation of aspirin.

PART-II

Qualitative analysis: Separation of binary mixtures, identification of functional groups and preparation of suitable solid derivatives

REFERENCES

1. A Text book of practical organic chemistry – A. I. Vogel Vol. I
2. Practical Organic Chemistry – Mann & Saunders
3. Manual of Organic Chemistry – Dey and Seetharaman
4. An introduction to practical organic chemistry – Robert, Vingrove etc.
5. Semimicro qualitative organic analysis by Cheronis, Entrikin and Hodnet
6. J. N. Guthru & R. Kapoor, Advance experimental chemistry, S. Chand Company, New Delhi, 1991
7. R. K. Bansal, Laboratory Manual of Organic Chemistry, New PGE International (P) Ltd. London, 3rd edition, 1996
8. N. K. Visno, Practical Organic Chemistry, New PGE International (P) Ltd. London, 3rd edition, 1996

PHYSICAL CHEMISTRY PRACTICALS

(120 HOURS)

PART-I

1. Study of kinetics of hydrolysis of an ester using HCl/H_2SO_4 at two different temperatures, determination of rate constants and energy of activation.
2. Study of kinetics of reaction between $K_2S_2O_8$ and KI, first order, determination of rate constants at two different temperatures and Ea.
3. Study of kinetics of reaction between $K_2S_2O_8$ and KI, second order, determination of rate constant and Ea.
4. Conductometric titration of a mixture of HCl and CH_3COOH against NaOH.
5. Conductometric titration of a mixture of HCl, CH_3COOH and $CuSO_4$ against NaOH.
6. Potentiometric titration of KI vs $KMnO_4$ solution.
7. Determination of dissociation constant of a weak acid by potentiometric method.
8. Potentiometric titration of $AgNO_3$ vs KCl.
9. To obtain the absorption spectra of coloured complexes, verification of Beer's law and estimation of metal ions in solution using a spectrophotometer.

10. Spectrophotometric titration of $FeSO_4$ against $KMnO_4$.
11. Determination of heat of solution of benzoic acid/salicylic acid by variable temperature method (graphical method).
12. Thermometric titration of an acid with a base.
13. Determination of molecular weight of a compound using Bekmann's cryoscopic method using benzene or/and water as solvent.
14. Potentiometric titrations of (a) Fe(II) Vs Ce(IV) (b) Fe(II) Vs V(V).
15. Kinetics of photodegradation of indigocarmine (IC) using ZnO/TiO_2 as photocatalyst and study the effect of [ZnO]/[TiO_2] and [IC] on the rate of photo degradation.
16. Conductometry –To determine the degree of hydrolysis and hydrolysis constant of aniline hydrochloride.
17. Conductometric titration of potassium iodide with mercuric perchlorate.
18. Determination of the molecular weight of a polymer material by viscosity measurements (polyvinyl alcohol/polystyrene/cellulose acetate/methyl acrylate).

PART-II

1. Analysis of a binary mixture by measurement of refractive index.
2. Determination of degree of association of benzoic acid in benzene by distribution method.
3. Binary analysis of two miscible liquids by viscometric method.
4. To study the salt effects on kinetics of reaction between $K_2S_2O_8$ and KI.
5. Study of kinetics of reaction between CAT and indigocarmine spectrophotometrically and determination of rate constant.
6. Determination of energy of activation for the bromide-bromate reaction.
7. Conductometric titration of sodium sulphate against barium chloride.
8. Determination of equivalent conductance at infinite dilution of a strong electrolyte and verification of Onsager equation.
9. Determination of dissociation constant of a weak electrolyte by conductivity method.
10. Potentiometric titration of a mixture of halides (KCl+KBr, KCl+KI and KBr+KI) against $AgNO_3$.
11. pH titration of (a) (CH_3COOH+HCl) Vs NaOH (b) $CuSO_4$ Vs NaOH and (c) CH_3COOH Vs NaOH and determination of Ka.
12. Determination of redox potential and estimation of Fe^{2+} ions by potentiometric method.
13. Determination of partial molar volume of (a) NaCl-H_2O and (b) C_2H_5OH-H_2O systems.
14. G.M. Counter –determination of G.M. plateau and dead time.
15. Verification of inverse square law using gamma emitter.
16. Kinetics of acid hydrolysis of an ester and study of effect of dielectric constant of the medium (using CH_3OH).
17. Conductometric titration of formic acid/oxalic acid against NaOH and NH_4OH.
18. Conductometric titration of orthophosphoric acid against NaOH.

REFERENCES

1. Practical Physical Chemistry – A.J. Findlay.
2. Experimental Physical Chemistry –F. Daniels et al.
3. Selected Experiments in Physical Chemistry – Latham.
4. Experiments in Physical Chemistry – James and Prichard.
5. Experiments in Physical Chemistry – Shoemaker.

6. Advanced Physico-Chemical Experiments –J. Rose.
7. Practical Physical Chemistry –S.R. Palit.
8. Experiments in Physical Chemistry – Yadav, Geol Publishing House.
9. Experiments in Physical Chemistry – Palmer.
10. Experiments in Chemistry –D.V. Jahagirdar, Himalaya Publishing House, Bombay, (1994).
11. Experimental Physical Chemistry –Das. R.C. and Behera B, Tata Mc Graw Hill, (1983).
12. Instrumental Methods in Chemical Analysis, Ewing. G.W, Mc Graw Hill, (1960).
13. Experiments in General Chemistry, CNR Rao and G.C. Agarwal, Affiliated East-West Press, (1966).
14. Polarography – Kolthoff and Lingane.

SECOND SEMESTER

CH 201 – SEPARATION TECHNIQUES

[48 HOURS]

UNIT-I

Solvent extraction*:* definition, types, principle and efficiency of extraction, sequence of extraction process, factors affecting extraction-pH, oxidation state, modifiers, synergistic, masking and salting out agents, techniques-batch and continuous extraction, applications.

Fundamentals of chromatography*:* General description, definition, terms and parameters used in chromatography, classification of chromatographic methods, criteria for selection of stationary and mobile phase-nature of adsorbents, factors influencing the adsorbents, nature and types of mobile phases and stationary phases.

Elution chromatography: Theories-plate theory; rate theory, band broadening-eddy diffusion, longitudinal diffusion and resistance to mass transfer, column efficiency-plate theory and rate theory approach, Van Deemter's equation and its modern version, optimization column performance, interrelationships-capacity factor, selectivity factor, column resolution, distribution constant and applications of conventional column chromatography, advantages and limitations.

[16 HOURS]

UNIT-II

Paper chromatography (PC): Definitions, theory and principle, techniques; one, two-dimensional and circular PC, mechanism of separation, structure of cellulose and types of paper, methodology-preparation of sample, choice of solvents, location of spots and measurement of RF value, factors affecting RF values, advantages and applications.

Thin-layer chromatography (TLC)*:* Definition, mechanism, efficiency of TL plates, methodology-selection of stationary and mobile phases-preparation of plates, spotting, development, identification and detection, reproducibility of RF values, comparison of TLC with high performance thin-layer chromatography, paper chromatography and column chromatography. Qualitative and quantitative analysis.

Gas chromatography (GC): Principle, comparison of GSC and GLC, instrumentation columns-packed and tubular, study of detectors-thermal conductivity, flame ionization, electron capture and mass spectrometry, factors affecting separation, applications.

High pressure liquid chromatography (HPLC)*:* Apparatus, pumps, column packing, characteristics of liquid chromatographic detectors-UV, IR, refractometer and fluorescence detectors, advantages and applications.

Ion-exchange chromatography(IEC): Definitions, requirements for ion-exchange resin, synthesis and types of ion-exchange resins, principle, basic features of ion-exchange reactions, resin properties-ion-exchange capacity, resin selectivity and factors affecting the selectivity, applications of IEC in preparative, purification and recovery processes.

Exclusion chromatography*:* Theory and principle of size exclusion chromatography, experimental techniques for gel-filtration chromatography (GFC) and gel-permeation chromatography (GPC), materials for packing-factors governing column efficiency, methodology and applications. **[16 HOURS]**

UNIT-III

Affinity chromatography*:* Definitions, separation mechanism-matrices, matrix activation, role of spacer arms and applications.

Ultracentrifugation*:* Principle sedimentation constant, sedimentation equilibrium, sedimentation velocity, methodology and applications.

Capillary electrophoresis*:* Overview, types, the basis for electrphoretic separations, migration rates and plate heights, electroosmotic flow, instrumentation, capillary zone electrophoresis, capillary gel electrophoresis, capillary isoelectrophoresis, capillary isoelectric focusing.

Capillary electrochromatography*:* Packed column electrochromatography, micellar electrokinetic capillary chromatography and applications.

Supercritical fluid chromatography*:* Properties of supercritical fluids, instrumentation and operating variables, comparison of supercritical to other types of chromatography, applications.

Supercritical fluid extraction: Advantages of supercritical fluid extraction, instrumentation, supercritical fluid choice, off-line and on-line extractions, typical applications of supercritical fluid extraction. **[16 HOURS]**

REFERENCES

1. Fundamental of Analytical Chemistry, D.A. Skoog, D.M. West, Holler and Crouch 8th edition, 2005, Saunders College Publishing, New York.
2. Analytical Chemistry, G.D. Christian, 5th ed., 2001 John Wiley & Sons, Inc, India.
3. Quantitative Analysis, R.A. Day and A.L. Underwood, 6th edition,1993 prentice Hall, Inc. New Delhi.
4. Vogel's Textbook of Quantitative Chemical Analysis, J. Mendham, R.C. Denney, J.D. Barnes and M.J.K. Thomas, 6th edition, Third Inidan Reprint.2003 Pearson Education Pvt. Ltd., New Delhi.
5. Analytical Chemistry Principles, John H. Kennedy, 2nd edition, Saunders College Publishing, California, 1990.

CH 202 – COORDINATION CHEMISTRY

[48 HOURS]

UNIT-I

Preparation of coordination compounds: Introduction, Preparative methods- simple addition reactions, substitution reactions, oxidation-reduction reactions, thermal dissociation reactions, reactions of coordinated ligands, the trans effect, other methods. Geometries of metal complexes of higher coordination numbers (2-12).

Stability of coordination compounds: Introduction, Stepwise and overall stability constants of coordination compounds, factors influencing the stability of metal complexes with reference to the nature of metal ion and ligand, the Irving-William series, chelate effect. Theoretical aspects of the determination of stability constants of the coordination compounds by spectrophotometric, pH metric, and polarographic methods.

Crystal Field Theory: Salient features of CFT, d-orbital splitting in octahedral, tetrahedral, square planar and tetragonal complexes, measurement of 10Dq. Spectrochemical series, short comings of CFT. **[16 HOURS]**

UNIT-II

Experimental evidences for covalence and adjusted CFT. MOT applied to octahedral, tetrahedral and square planar complexes without and with pi-bonding. M.O.energy diagrams for octahedral complexes with sigma –ligands having pi- systems. Jahn –Teller effect.

Electronic absorption spectra of transition metal complexes: Introduction, selection rules,electronic–dipole transitions, magnetic-dipole transitions, term symbols for d^n ions, effects of spin orbit coupling, energy level diagrams, Orgel and Tanabe-Sugano diagrams, charge-transfer transitions.

Magnetic properties of transition metal complexes: Introduction, magnetic susceptibility and its measurements, spin cross over systems, ferromagnetism and antiferro magnetism. **[16 HOURS]**

UNIT-III

Reaction kinetics of coordination compounds: Introduction, electron transfer reactions: Outer-sphere reactions, the Marcus theory, ligand-bridged inner sphere reactions doubly-bridged inner-sphere transfer, one electron and two electrons transfers, non-complementary reactions. Ligand exchange via electron exchange. Mechanisms of ligand substitution reactions-general considerations, substitution reactions of square planar and octahedral complexes. Base-catalyzed hydrolysis of cobalt(III) ammine complexes.

Metal-metal bonding: Evidences and factors favouring of M-M bonding, bi, tri, tetra, penta and hexa nuclear metal clusters.

Thermodynamic and related aspects of ligand fields: Hydration, ligation and lattice energies.

[16 HOURS]

REFERENCES

1. Advanced inorganic chemistry, (5^{th} edition) – F.A. Cotton and G. Wilkinson: John Wiley and sons 1988.
2. Inorganic chemistry (3^{rd} edition) – J.E. Huheey: Harper and Row, N.Y. 1983.
3. Modern aspects of Inorganic chemistry (4^{th} edition) – H.J., Emeleus and A.G. Sharpe: UBS 1989.

4. Coordination chemistry – S.F.A. Kettle, (1969) – Thomas Nelson and Sons Ltd., London.
5. Physical Inorganic Chemistry- A Coordination Chemistry Approach – S.F.A.Kettle, Spektrum, Oxford, 1996.

CH 203 – SYNTHETIC ORGANIC CHEMISTRY

[48 HOURS]

UNIT-I

Reductions: Catalytic hydrogenations (homogeneous and heterogeneous)-catalysts, solvents, equipment and reduction of functional groups, catalytic hydrogen transfer reactions, Wilkinson catalyst, Bakers yeast, $LiAlH_4$, $NaBH_4$, metal dissolving reactions (Birch reduction), Leukert reaction (reductive amination), diborane, Meerwein-Pondorf-Varley reduction, Wolf-Kishner reduction, Clemensen reduction.

Oxidations: Oxidation with chromium and manganese compounds (CrO_3, $K_2Cr_2O_7$, PCC, PDC, Sarret reagent, Jones reagent, MnO_2, $KMnO_4$), oxygen (singlet and triplet), ozone, peroxides and peracids, lead tetra acetate, periodic acid, OsO_4, SeO_2, NBS, chloramine-T, Sommelet oxidation, Oppenauer oxidation. **[16 HOURS]**

UNIT-II

Reagents in organic synthesis: Use of following reagents in organic synthesis and functional group transformations: Gilmann reagent, dicyclohexyl carbodiimide, DDQ, trimethylsilyl halides, trimethylsilyl cyanides, dithianes, TBDMS-chloride, phase transfer catalyst, crown ethers, cyclodextrins, Fenton's reagent, triphenyl phosphine, Aluminium oxide, Ziegler-Natta catalyst, diazomethane, stannous chloride, Lawson reagent, thiourea, sharpless epoxidation, Woodward and Prevost hydroxylation, Peterson reaction, metal carbonyls. **[16 HOURS]**

UNIT-III

Design and synthesis:

Protecting groups: protection of hydroxyl, carboxyl, carbonyl, thiol and amino groups. Illustration of protection and deprotection in synthesis.

Aldol and related reactions: Keto-enol tautomerism, mechanism and synthetic applications of aldol condensations, Claisen reaction, Schmidt reaction, Perkin reaction, Knovenogal, benzoin, Stobbe condensation, Darzens Glysidic ester condenasation, Cannizaro reaction, Tschenko reaction, Michael addition, Robinson's annulation reactions.

Introduction to disconnection approach. Basic principles and terminologies used in disconnection approach. One group C-X and two group C-X disconnections. Synthons and synthetic equivalents.

Retrosynthesis: Benzofurans, p-methoxy acetophenone, saccharine, α-bisabolene, nuciferal, penicillin-V, cantheridin, estrone and cubane. **[16 HOURS]**

REFERENCES

1. H. Pine, Hendrickson, Cram and Hammond, Organic Chemistry, Mac Grow Hill, New York, 1987.
2. Organic Chemistry – Morrison & Boyd
3. I. Finar, Organic Chemistry, ELBS Longmann, Vol. I & II, 1984

4. J. March, Advanced Organic Chemistry, Willey Interscience, 1994.
5. E. S. Gould, Mechanism Mechanism and Structure in Organic Chemistry, Halt, Rinhart & Winston, New York, 1964.
6. F. A. Carey and Sundberg, Advanced Organic Chemistry – Part A & B, 3rd edition, Plenum Press, New York, 1990.
7. Comprehensive Organic Synthesis – B. M. Trost and I. Fleming series, Pergamon Press, New York, 1991.
8. A Guide book to mechanism in organic chemistry – Petersyke
9. S. K. Ghosh, Advanced General Organic Chemistry, Book and Alleied (P) Ltd, 1998

CH 204 – THERMODYNAMICS AND STATISTICAL MECHANICS

[48 HOURS]

UNIT-I

Concepts of entropy and free energy: Entropy as a measure of unavailable energy. Entropy change during spontaneous process. Helmholtz and Gibbs free energies. Thermodynamic criteria of equilibrium and spontaneity. Variation of free energy with temperature and pressure. Maxwell's relations, Van't Hoff's reaction isotherm and isochore, Gibbs-Helmholtz equation. Determination of free energy changes. Nernst heat theorem and Third law of thermodynamics-calculation of absolute entropies.

Partial molar properties: Partial molar volumes and their determination by intercept method and from density measurements. Chemical potential and its significance. Variation of chemical potential with temperature and pressure. Formulation of the Gibbs Duhem equation. Thermodynamic derivation of the law of mass action. Derivation of Duhem-Margules equation. **[16 HOURS]**

UNIT-II

Fugacity: Determination of fugacity of gases. Variation of fugacity with temperature and pressure. Activity and activity coefficients. Variation of activity with temperature and pressure. Determination of activity coefficients by vapour pressure, depression in freezing point, solubility measurements and by electrical methods.

Thermodynamics of dilute solutions: Raoult's law, Henry's law. Ideal and non-ideal solutions. Discussion and derivation of the laws of osmotic pressure, cryoscopy and ebullioscopy. Determination of molecular weights. Donnan membrane equilibrium: Thermodynamic treatment using the concept of chemical potentials. Heat capacity of solids, Einstein and Debye heat capacity equations, characteristic temperature and its significance.

Phase Rule Studies: Thermodynamic derivation of phase rule, application of phase rule to the two component systems, simple eutectic type, compound formation with congruent melting point and incongruent melting points, systems involving the formation of a continuous series of solid solutions, Roozeboom's classification. Application of phase rule to three component systems. Systems of three liquids, systems of two salts and water. **[16 HOURS]**

UNIT-III

Statistical mechanics: Introduction, thermodynamic probability relation between entropy and thermodynamic probability, principle of equipartition of energy, Maxwell-Boltzmann distribution equation, partition function, translational, rotational and vibrational partition functions, evaluation of molar entropies, entropy of monatomic gas (Sackur-Tetrode equation). Evaluation of internal energy, enthalpy, Helmholtz and Gibbs free energies, equilibrium constant, partition functions of atoms and diatomic molecules**.**

Distribution equations – Bose-Einstein and Fermi-Dirac distribution equations. Free energy function and its use in evaluating the equilibrium constant, entropy of water and hydrogen. **[16 HOURS]**

REFERENCES

1. Thermodynamics for chemists by S. Glasstone, Affiliated East-west press, New Delhi, (1965).
2. Chemical Thrmodynamics by I.M. Klotz, W.A. Benzamin Inc. New York, Amsterdam, (1964).
3. Basic Physical Chemistry by W.J. Moore, Prentice Hall of India Pvt. Ltd., New Delhi, (1986).
4. Text book of Physical Chemistry by Samuel Glasstone, MacMillan Indian Ltd., (II edition), (1974).
5. Theoretical chemistry by S. Glasstone.
6. Statistical themodynamics by B.C. Meclelland, Chapman and Hall, London (1973).
7. Elementary statistical thermodynamics by N.D. Smith Plenum Press, NY (1982).
8. Elements of classical and statistical thermodynamics by L.K. Nash, Addison-Wesley (1970).
9. Statistical thermodynamics by I.M. Klotz.
10. Introduction to Statistical Thermodynamics by M. Dole, Prantice-Hall, (1962).

CH 204 – CHEMICAL SPECTROSCOPY - I

[48 HOURS]

UNIT-I

Microwave spectroscopy: Classification of the molecules based on rotation - Linear, symmetric, spherical and asymmetric top molecules (HCl, HCN, H_2O, BCl_3, CH_4 and CH_2 = CHCl). Pure Rotation Spectra of Diatomic Molecules - Rigid rotor model, energy levels , rotational quantum number and the selection rule. Effect of non-rigid rotation. Determination of moment of inertia and bond length of diatomic molecules usung rotational spectra.. Effect of isotopic substitution on rotation spectra. Relative intensities of the spectral lines. Rotation spectra of polyatomic molecules (BCl_3, OCS and CH_3F). Moment of inertia expression for linear and non-linear molecules. Experimental techniques - Microwave spectrometer. Applications - Principles of determination of Bond length and Moment of inertia from Rotational Spectra. Stark effect in rotation spectra and determination of dipole moments.

Raman spectroscopy: Introduction, Raman and Rayleigh scattering, stokes and anti-stokes lines, polarization of Raman lines, depolarization factor, polarizability ellipsoid. Theories of Raman spectra-classical and quantum theory. Rotation, vibration and rotation - vibration Raman spectra. Comparison of Raman and IR spectra, rule of mutual exclusion principle. Advantages of Raman spectra. Molecular data bond length and vibration determined by Raman spectroscopy.

[16 HOURS]

UNIT - II

Vibration spectroscopy*:* Vibration of diatomic molecules, the energy curves for simple harmonic oscillator – vibration spectra. Effects of anharmonic oscillation – the diatomic vibrating rotator-vibration rotation spectra of carbon monoxide. Expressions for fundamental and overtone frequencies.

Vibration of polyatomic molecules – The number of degrees of freedom of vibration and their symmetry- overtones and combination frequencies - Influence of rotation on the spectra. Parallel and perpendicular vibrations (CO_2 and H_2O). Fundamental, overtone, combination and difference bands. Fermi resonance. Force constant, its determination and significance. Theory of infrared absorption and theoretical group requency. Intensity of absorption band and types of absorptions. Correlation chart. Important spectral regions- Hydrogen stretching region, Triple bond region, double bond region and "Fingerprint region". Applications : Structure of small molecules: XY_2 – linear or bent, XY_3 – planar or pyramidal. Coordination chemistry (Aquo, amino, nitrite, thiocyanate) – change in symmetry on coordination (nitrate, carbonate and sulphate complexes) – organometallic compounds – geometrical isomers and Jahn-Teller effect. Organic compounds – Structure determination and the characteristic group frequencies. Factors affecting the group frequency – Physical state, vibrational coupling, electrical effect, hydrogen bonding, steric effect and ring strain. Interpretation of IR spectra for qualitative identification of polymers. **[16 HOURS]**

UNIT - III

UV-VIS Spectroscopy (outer shell electronic spectroscopy): Quantitative aspects of absorption-Beer's law. Terminology associated with absorption measurements. Limitations of the law: Real, Chemical, instrumental and personal. Theory of molecular absorption. Vibration-rotation fine structure of electronic spectra. Types of absorption bands: $n \rightarrow \pi^x$, $\pi \rightarrow \pi^x$, $n \rightarrow \sigma^x$, $\sigma \rightarrow \sigma^x$, C-T & ligand field. Empherical rules for predicting the wavelength of maximum absorption: - Olefins, conjugated dienes, cyclic trienes and polyenes- α,β-unsaturated aldehydes and ketones-benzene and substituted benzene rings. Basic components of instrumentation, single and double beam designs. Applications: Qualitative and Quantitative analysis of binary mixtures, measurement of dissociation constants of acids and bases, determination of molecular weight, photometric titrations, Determination of stoichiometry and stability of the complexes and kinetic studies. **[16 HOURS]**

REFERENCES

1. Symmetry in Chemistry, - H. Jaffe and M. Orchin, John Wiles, New York, (1965).
2. Symmetry in Molecules, - J.M. Hollas, Chapman & Hall Ltd., London, (1972).
3. Chemical Applications of group theory, - F.A. Cotton, Wiley Eastern Ltd., 2nd Edition, New Delhi, (1971).
4. Group theory and Symmetry in Chemistry, -G. Raj, A. Bhagi and V. Jain, Krishna Prakashan Media (P) Ltd., Meerut, (1998).

CH 206 – PHOTOCHEMISTRY AND RADIATION CHEMISTRY

[48 HOURS]

UNIT-I

Photochemistry: Introduction to photochemistry, quantum yield and its determination, factors affecting quantum yield, experimental technique in photochemistry, Actinometry -Uranyloxalate and potassium ferrioxalate actinometers, acetone and diethylketone actinometers. Term symbols and significance. Photosensitization: by mercury, dissociation of H_2, sensitized isomerization. Photodimerization of anthracene, photochemical kinetics of: Decomposition of HI, CH_3CHO; formation of HCl, HBr and $COCl_2$; Chlorination of Chloroform. Photodegradation: Photocatalyst – ZnO, TiO_2, Principle, Application of ZnO/TiO_2 in the photo degradation of dyes (IC), pesticides (DDT) and in industrial effluents. Effect of photo degradation on COD value.

Direct spectroscopic identification of primary processes, use of free radical traps in the determination of primary photodecomposition modes. Photophysical properties: Fluorescence, characteristics of fluorescence, resonance fluorescence, sensitized fluorescence, quenching of fluorescence, phosphorescence, characteristics, chemiluminescence – theory and applications. Photochemistry of coordination compounds **[16 HOURS]**

UNIT-II

Photochemistry and concerted reactions: Introduction, light absorption and electronic transitions, Jablonski diagram, intersystem crossing, energy transfer, sensitizers, quenchers
Photochemistry of olefins, conjugated dienes, aromatic compounds, ketones, enones, photooxidations, photoreductions, Norrish type I and II reactions, Paterno-Buchi reaction, Barton reaction, Di-pi-rearrangements

Pericyclic reactions:

Electrocyclic reactions: stereochemistry, symmetry and Woodward-Hofmann rules for electrocyclic reactions, FMO theory of electrocyclic reactions, correlation diagram for cyclobutadiene and cyclohexadiene systems.

Cycloaddition reactions: [2+2], [3+2] and [4+2] cycloadditions, analysis by FMO and correlation digram method.

Sigamatropic reactions: Classification, stereochemistry and mechanisms. **[16 HOURS]**

UNIT-III

Radiation chemistry: Introduction, units, interaction of electromagnetic radiation with matter, G-value, LET of radiation, dosimetry, characteristics, Fricke and Ceric sulphate dosimeters.Radiolysis - water, cysteine, methane, carbon tetrachloride, chloroform, benzene and biphenyl.

Radioisotopes as tracers, use of isotopic tracers in the elucidation of reaction mechanism, structure determination and solubility of sparingly soluble substances. Isotope exchange reactions, quantitative exchange law, isotopic dilution method, neutron activation analysis, radiometric titration, ^{14}C dating, Medical applications of isotopic tracers. Hazards in radiochemical work and radiation protection.

[16 HOURS]

REFERENCES

1. Photochemistry - Calvert & Pitts, Wiley, New York, (1966).
2. Advances in Photochemistry - Rohatgi Mukherjee.
3. Principle and applications of Photochemistry – R.P. Wayne, Elsevier, New York, (1970).
4. Photochemistry, Paul Suppan, RSC, London, (1944).
5. Dupey and Chapmann, Molecular reactions and Photochemistry, Prenctic Hall- International, Tokyo, 1972.
6. Introduction to physical organic chemistry – Kosower
7. Molecular orbital calculations – J. D. Roberts
8. N. J. Turro, Modern molecular photochemistry, The Benzamin Cummings Publishing Co. Ltd, Menlo Park, 1978.
9. K. Yates, Huckel's Molecular Orbital Theory, Academic Press, New York, 1978.
10. T. L. Gilchrist & R. C. Storr, Organic reaction and orbital symmetry, Cambridge Univ. Press, London, 1979.
11. D. C. Neckers, Mechanistic Organic Photochemistry, Reinhaold, New York, 1967.
12. Source book on atomic energy by S. Glasstone, 3rd edition, Van Nostrand (1967).
13. Nuclear chemistry by Friendlander and Kennedy, John Wiley and Sons (1987).

14. Essentials of nuclear chemistry by H.J. Arnikar, Eastern Wiley (1990).
15. Radiation Chemistry by A.J. Swallow, Longmann (1973).
16. An introduction to radiation chemistry, Spinks and Woods.
17. Fundamentals of radiochemistry by D.D. Sood, A.V.R. Reddy and N. Ramamoorthy, Indian Association of Nuclear Chemists and Allied Scientist 2nd edition (2004).

SECOND SEMESTER PRACTICALS

ANALYTICAL/INORGANIC CHEMISTRY PRACTICALS
ORGANIC/PHYSICAL CHEMISTRY PRACTICALS

[120 HOURS]

Experiments are as in First semester. Every student will carry out experiments on a rotation basis in the FIRST and SECOND SEMESTERS.

THIRD SEMESTER

CH 301 – ELCTROANALYTICAL, OPTICAL AND THERMAL METHODS OF ANALYSIS

[48 HOURS]

UNIT-I

Electroanalytical methods: Introduction to electro analytical methods.

Potentiometry: Fundamentals of potentiometry. indicator and ion-selective electrodes. Membrane electrodes. Glass electrode for pH measurement, glass electrodes for cations other than protons. Liquid membrane electrodes, solid state ion selective detectors and biochemical electrodes. Applications of potentiometry. Direct potentiometric measurements-determination of pH and fluoride.

Redox and potentiometric titrations- Balancing redox reactions, calculation of the equilibrium constant of the reaction, titration curves, visual end point detection. Redox indicators-theory, working and choice. Potentiometric end point dection. Applications of redox titrations. Sample preparation-prereduction and preoxidation.

Electrogravimetric analysis: Theory, apparatus, cell processes, deposition and separation, electrolytic separation of metals, applications.

Coulometry: General discussion, coloumetry at controlled potential, apparatus and general technique, applications coloumetric titrations (amperometric coulometry)-principles, apparatus, comparision of coulometric titrations with conventional titrations, automatic coulometric titrations, applications.

Voltammetry: Fundamentals of voltammetry. **Cyclic voltammetry:** Principles and applications. **Stripping analysis:** Stripping voltammetry-basic principles, electrodes used for stripping analysis, apparatus for stripping analysis, applications, determination of lead in water voltammetry with micro electrodes. **[16 HOURS]**

UNIT-II

Flame photometry and Atomic absorption spectrometry : Energy level diagrams –atomic absorption spectra. Flame characteristics. Flame atomizers and electrothermal automization. Comparision of spectral interferences, chemical and physical interferences in FP and AAS. Use of organic solvents. Quantitative techniques–calibration curve procedure and the standard addition technique. Typical commercial instruments for FP and AAS. Applications. Qualitative analysis and quantitative evaluations. Relative detectabilities of atomic absorption and flame emission spectrometry.

Molecular luminescence spectrometry: Theoretical basis for fluorescence and phosphorescence.

Singlet and triplet excited states . Variables affecting luminescences – Quantum efficiency, transition

types, structure and structural rigidity, temperature and solvent effects, effect of pH, dissolved oxygen and concentration effect. Excitation spectra *vs* emission spectra. Fluorescence instrumentation – fluorometers and spectrofluorometers. Sensitivity and selectivity. Modification necessary to measure phosphorescence. Comparision of fluorescence and phosphorescence. General scope of applications of luminescence. **[16 HOURS]**

UNIT-III

Thermal methods of analysis (TGA): Principle-factors affecting the TGA data. Instrumentation – balance, furnace, instrument control/data handling-applications.
Differential thermal analysis (DTA): Theory – variables affecting the DTA curves. Instrumentation, general principles, applications.
Differential scanning calorimetry (DSC): Differences between DTA and DSC. Instrumentation-power compensated DSC, Heat flux DSC. Applications. **[16 HOURS]**

REFERENCES

1. Fundamental of Analytical Chemistry, D.A. Skoog, D.M. West, Holler and Crouch 8th edition, 2005, Saunders College Publishing, New York.
2. Analytical Chemistry, G.D. Christian, 5th ed., 2001 John Wiley & Sons, Inc, India.
3. Quantitative Analysis, R.A. Day and A.L. Underwood, 6th edition,1993 prentice Hall, Inc. New Delhi.
4. Vogel's Textbook of Quantitative Chemical Analysis, J. Mendham, R.C. Denney, J.D. Barnes and M.J.K. Thomas, 6th edition, Third Indian Reprint.2003 Pearson Education Pvt. Ltd., New Delhi.
5. Analytical Chemistry Principles, John H. Kennedy, 2nd edition, Saunders College Publishing, California, 1990.
6. Instrumental Methods of Analysis by H.H. Willard, L.L. Merritt and J.A. Dean, 7th Edition, (1988).

CH 302 – ORGANOMETALLIC CHEMISTRY

[48 HOURS]

UNIT-I

Organometallic Chemistry: Introduction, 16 and 18 electrons rule, classification of organometallic compounds by bond type, nomenclature.
Chemistry of organometallic compounds: Synthesis and reactions of organomagnesium (Grignard reagent), organomanganese, organoaluminium, organotin, organozinc, organolithium (n-BuLI, PhLi) reagents.

Metal Carbonyl Complexes: Preparation, structure, chemical bonding in metal carbonyls, physical evidence related to M-CO bonding. Preparation of anionic metal carbonyl complexes and substituted metal carbonyl complexes.
Cyclopentadienyl Metal Complexes: Preparation and structures of cyclopentadienyl metal complexes. M.O diagram for ferrocene. Reactions and aromaticity of ferrocene. **[16 HOURS]**

UNIT – II

Metal-arene Complexes: Methods of preparation of arene complexes, reactions of metal-arene complexes, structure and bonding in arene-metal complexes.
Heterocyclic sandwich compounds: Preparation and properties.
Olefin-transition metal complexes: Methods of preparation, structure and bonding in metal olefin complexes.
Conjugated diolefins and related metal complexes: Preparation, structure and bonding.
Acetylene and acetylene derived metal complexes: Preparation, structure and bonding in acetylene complexes. Reactions of coordinated acetylene.
Pi-allylic metal complexes: Preparation of complexes containing allylic ligands, structure and bonding. **[16 HOURS]**

UNIT-III

Homogeneous Catalysis: Introduction, properties of catalysis, types of reactions in homogeneous catalysis, hydrogenation of olefins, isomerization of olefins, oxo-process, Wacker process, Monsanto acetic acid process. Monsanto L-Dopa synthesis, water gas shift reaction, carbonylation, template synthesis, alkene hydrosilation.
Herterogeneous Catalysis: Introduction, Fischer-Tropsch reaction, Ziegler-Natta catalysis.
Biological applications and environmental aspects of organometallic compounds: Introduction, organometallics in medicine, agriculture, horticulture and environmental aspects. **[16 HOURS]**

REFERENCES

1. Inorganic Chemistry - F.A. Cotton and G. Wilkinson (2^{nd} edn).
2. Inorganic Chemistry Principles and Structure –J. Huheey.
3. Organometallic Chemistry – R.C. Mehrothra and A. Singh.
4. Fundamental Transition metal Organometallic Chemistry – Charles M. Lukehart.
5. Inorganic chemistry- Purcell and Kotz.
6. J. March, Advanced Organic Chemistry, Willey Interscience, 1994.
7. Comrehensive Organic Synthesis, – Trost series, Pergamon Press, New York, Vol. 1, 1991.
8. R. Norman and J. M. Coxon, Principles of organic synthesis, 2^{nd} edition, Replika Press Pvt. Ltd., India, 2005.

CH 303 – HETEROCYCLIC CHEMISTRY, MOLECULAR REARRANGEMENT AND SYNTHETIC DRUGS [48 HOURS]

UNIT-I

Chemistry of heterocyclic compounds: Nomenclature of heterocyclic systems, Synthesis and typical reactions of furan, pyrrole, thiophene, indole, pyridine, quinoline, isoquinoline, pyrone, coumarin, chromones, pyrimidines and purines. Synthesis and synthetic applications of azirines and aziridines, oxazolines, and isoxazole. **[16 HOURS]**

UNIT-II

Molecular rearrangements: Introduction.
Carbon-to carbon migrations: Pinacol-pinacolone, Wagner-Meerwein, Benzidine, Demjanov, Benzilic acid, Favorskii, Fries, Cope, Claisen rearrangement, von Richter raction.
Carbon-to nitrogen migrations: Hofmann, Curtius, Lossen, Schmidt and Beckmann rearrangement.

Miscellaneous rearrangement: Stevens, Sommelet-Hauser, Wittig, Smiles, Neber, Japp-Klingermann rearrangement, Baeyer-Villeger rearrangement. **[16 HOURS]**

UNIT-III

Synthetic Drugs: Introduction, chemotherapy, pharmacodynamics, metabolites and antimetabolites, agonists and antagonists.

A general study of the following class of drugs.

1. Sulpha drugs: sulphonamides, sulphamethoxazole.
2. Antipyretics: Aspirin, paracetamol, phenacetin, novalgin.
3. Antimalarials: Qunine, chloroquine.
4. Hypnotics, analgesics and sedatives: Phenobarbital, hlorodiazopoxide, meprobamate.
5. Antihistamines: chlorphenramine.
6. Stimulants: caffeine.
7. Antineoplastic: 5-flurouracil and chlorambucil.
8. Antibiotics: Introduction, structure, and synthesis of streptomycin, chloromycetin and tetracyclines.

[16 HOURS]

REFERENCES

1. H. Pine, Hendrickson, Cram and Hammond, Organic Chemistry, Mac Grow Hill, New York, 1987.
2. Organic Chemistry – Morrison & Boyd
3. I. Finar, Organic Chemistry, ELBS Longmann, Vol. I & II, 1984
4. J. March, Advanced Organic Chemistry, Willey Interscience, 1994.
5. E. S. Gould, Mechanism Mechanism and Structure in Organic Chemistry, Halt, Rinhart & Winston, New York, 1964.
6. F. A. Carey and Sundberg, Advanced Organic Chemistry – Part A & B, 3rd edition, Plenum Press, New York, 1990.
7. Heterocyclic Chemistry –Joule & Smith
8. Heterocyclic chemistry – Acheson
9. Burger's Medicinal Chemistry and drug discovery, Ed. Manfred, E. Wulf, Vol. I-IV, Jhon Wiley & Sons, 1995.
10. Pharmecutical Chemistry by G. R. Chatwal et al, Himalayan Publishing House, New Delhi.
11. Basic Principles of heterocyclic chemistry – L. A. Pacquette
12. Comprehensive heterocyclic chemistry –Kartritzky series, Pergamon Press, New York, 1984.

CH 304 – CHEMICAL KINETICS

[48 HOURS]

UNIT-I

Kinetics of complex reactions: Parallel, consecutive and reversible reactions. Determination of order of reaction. Arrhenius equation, energy of activation and its experimental determination. Simple collision theory-mechanism of bimolecular reaction. Lindemann's theory, Hinshelwood's theory for unimolecular reaction. Activated complex theory of reaction rate, classical thermodynamic treatment, partition function, statistical thermodynamic treatment. Kinetics of reactions in solution-Salt effects, effect of dielectric constant (single sphere and double sphere model), effect of pressure, volume and

entropy change on reaction rates. Cage effect with an example. Kinetics of heterogeneous reactions - Langmuir's theory, unimolecular and bimolecular surface reactions. **[16 HOURS]**

UNIT-II

Fast Reactions: Study of kinetics by flow techniques, equation for contact time, stopped flow and continuous flow methods. Relaxation method, equation for relaxation time, temperature jump and pressure jump methods, flash photolysis, pulse radiolysis and shock tube method.
Potential energy surface, theoretical calculation of energy of activation.
Chain reactions: Rice-Herzfeld mechanism for the thermal decomposition of acetaldehyde, Kinetics of explosive reactions, explosion limits (H_2 and O_2 reaction). Kinetics of autocatalytic and oscillatory chemical reactions, oscillatory chemical reaction of oxidation of malic acid by bromate ion catalyzed by Ce (III). Catalyzed and uncatalyzed reaction: Ru(III) catalyzed oxidation reaction of primary amines by chloramine –T in HCl medium. **[16 HOURS]**

UNIT-III

Kinetic methods of analysis: Analytical uses of reaction rates relative, basis of reaction rate methods, rate laws-first and second order reactions relative rates of reactions, analytical utility of first or psuedo first order reactions, determination of reaction rates, types of kinetic methods–differential methods, integral methods, multicomponent analysis-neglect of reaction of slow-reacting component, logarithmic extrapolation method, reaction rate method, applications-catalyzed reactions, measurement methods for catalyzed reactions, micro determination of inorganic species like iodide, selenium, cobalt & mercury in complex materials, determination of organic species, non-catalytic reactions. Applications of enzyme-catalysed reactions for the analysis of substrates-stoichiometric and rate methods, determination of urea, uric acid, blood glucose, galactose and blood alcohol, determination of enzymes-LDH, GOT and GPT.
A brief outline of IR, UV, NMR, Mass spectroscopy as tools for kinetic study.

[16 HOURS]

REFERENCES

1. Chemical Kinetics by K.J. Laidler.
2. Chemical Kinetics –Frost and Pearson.
3. Kinetics and Mechanism of Chemical Transformation by J. Rajaram and J.C. Kuriacose.
4. Chemical Kinetics –L.K. Jain.
5. Chemical Kinetics –Benson.
6. Elements of Physical Chemistry –Lewis and Glasstone.
7. Physical Chemistry by P.W. Atkins, ELBS, 4th Edition, Oxford University Press (1990)
8. Kinetics in Analytical Chemistry – H. B. Mark and G. A. rechnitz, Interscience Publishers, John Willey and Sons, New York.

CH 305 – CHEMICAL SPECTROSCOPY - II

[48 HOURS]

UNIT - I

NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY: General introduction. Theory of magnetic resonance - magnetic properties of nuclei, spin number and allowed transitions – classical description and Fourier Transform NMR. Population of nuclear magnetic energy levels - relaxation processes – factors affecting line width. Magnetic shielding – Chemical shift – standards employed – shielding mechanisms – chemical shift correlations. Spin-spin interactions – coupling constants and Factors influencing the coupling constant – splitting patterns – first order rules for predicting the band multipletes. Proton decoupling – Broad band decoupling, Off-Resonance Decoupling, Pulse decoupling and Nuclear Overhauser Enhancement. Simplification of complex spectra – Increased field strength, Spin decoupling or Double resonance and Contact – Shift reagents. Studies of nuclei other than protons –^{13}C, ^{19}F, ^{14}N and ^{31}P. Applications – identification, analysis of binary mixtures, Applications of NMR-structural diagnosis, conformational analysis, keto-enol tautomerism, determination of reaction velocities, H-bonding. Structure determination using ^{13}C-NMR, application of NMR to other nuclei. Two-dimensional NMR. Magnetic Resonance Imaging. **[16 HOURS]**

UNIT - II

Mass spectrometry: Principles, instrumentation, different methods of ionization. EI, CI, FD and FAB, Ion separators-single focusing separator with magnetic diffraction, double focusing analyzer, time-of-flight separator and quadrupole analyzer. Mass spectra – molecular ion, base peak, meta-stable peak. General rules for fragmentation pattern. Nitrogen rule, Hydrogen transfer rearrangement and McLafferty rearrangement. Mass spectral fragmentation of organic and inorganic compounds. Examples of mass spectral fragmentation of organic and inorganic compounds with respect to their structure determination. Applications: Identification of pure compounds, Molecular weight determination, Molecular formula from isotopic ratio, Structural information from fragmentation patterns, Evaluations of thermodynamic data, heats of sublimation and species in the vapour over high melting solids, appearance potentials and ionization potentials. **[16 HOURS]**

UNIT – III

ESR Spectroscopy: Basic principles – Intensity, width, position and multiple structure. General rules for the interpretation of the spectra. Zero field splitting and Kramer's degeneracy . Factors affecting the magnitude of 'g' value. Double resonance-ENDOR and ELDOR. Applications – study of free radicals, structure determinations, biological study, coordination compound and analytical applications.

Mössbauer Spectroscopy: Theoretical basis. Interpretation of Mössbauer Spectra – Isomer shift, Quadrupole splitting and Magnetic hyperfine structure, Time and temperature dependent effects. Instrumentation. Applications – structure deductions – $I_2Br_2Cl_4$, $Fe_3(CO)_{12}$.

NQR Spectroscopy: Energies of the quadrupole transitions, effect of magnetic field on the spectra, relationship between electric field gradient and molecular structure. Applications – interpretation of e^2Qq data. Structural information from NQR spectra. **[16 HOURS]**

REFERENCES

1. Spectroscopy by B. P. Straughan and S. Walker, John Wiley & Sons Inc., New York, Vol. 1 and 2, 1976.
2. Organic spectroscopy by William Kemp, ELBS Society, MacMillan, 1987.

3. Application of absorption spectroscopy of organic compounds by John R. Dyer, Prentic-Hall of India Private Ltd., New Delhi, 1974.
4. Organic spectroscopy by V. R. Dhani, Tata McGrow-Hall publishing compny Ltd., New Delhi, 1995.
5. Spectrometric identification of organic compounds, 4th edition, Robert M. Silverstein, G. Clayton Bassler and Terence C. Morrill, John Wiley & Sons Inc., New York, Vol. 1, 1981.
6. Interpretation of carbon-13 NMR spectra, F. W. Wehrli and T. Wirthlin, Heyden, London, 1976.
7. Analytical Chemistry Principles, John H. Kennedy, 2nd edition, Saunders College Publishing, California, 1990.
8. Instrumental Methods of Analysis, Hobart H. Willard, Lynne L. Merritt, Jr., John A. Dean & Frank A. Settle, Jr., 6th edition, CBS Publishers & Distributors, Delhi, 1986.
9. Physical Methods for Chemists by R. S. Drago, Saunders College Publishing, New York.
10. Quantitative Analysis, R.A. Day and A.L. Underwood, 6th edition, prentice Hall, Inc. 1999.
11. Principles of Instrumental Analysis, D.A. Skoog, F.J. Holler and T.A. Nieman, 5th edition, Thomson Asia Pvt. Ltd., Singapore, 1998.
12. Analytical Chemistry, G.D. Christian, 5th ed., John Wiley & Sons, Inc, India, 2001.
13. Structural methods in inorganic chemistry by E. A. V. Ebsworth, D. W. H. Rankin and S. Cradock.

CH CBCBS - I– GENERAL CHEMISTRY

UNIT-I

ANALYTICAL AND INORGANIC CHEMISTRY

Statistical Treatment of Analytical Data and Sampling: Limitations of analytical methods. Classification of errors-systematic errors-sources, effects and their reduction. Random errors-sources and distribution. Accuracy and precision.

Fundamentals of chromatography*:* General description - definition, terms and parameters used in chromatography (Rf-value, retention volume and time).Ion-exchange chromatography (IEC) and its application in separation of the components from the mixture.

Potentiometry and conductometry : Principle and Applications.

Ionic bond and covalent bond: Properties of ionic substances, structure of ionic crystals. Hybridization, VSEPR concept to explaining the structures of simple molecules.

Modern concepts of acids and bases: Arrhenius, Bronsted-Lowry, Lewis, Lux-Flood and solvent system concepts. Survey of essential and trace elements in biological system.

Correlation of general properties of d-block elements with f-block elements (electronic configuration and oxidation states). Industrial applications of some transition and non-transition elements. Crystal field splitting of d-orbitals in octahedral and tetrahedral complexes. **[15 HOURS]**

UNIT – II

CHEMICAL SPECTROSCOPY

Infrared Spectroscopy: Theory of infrared absorption. Types of absorption. Intensity of absorption bands. Number of fundamental vibrations and Theoretical group frequencies. Identification, interpretation of infrared spectra – Correlation chart, important spectral regions, characterization of functional groups and structure determinations – CO_2 and H_2O, CH_3COCH_3.

UV-Visible Spectroscopy: Introduction Absorption and transmission. Colour and chemical constitutions – chromophores and auxochromes Relationship between observed colur and absorption. Beer's law of absorption and its limitations. Applications: Qualitative and quantitative analysis, study of atmospheric pollutants.

^{1}H-NMR spectroscopy: Theoretical basis – Nuclear spin, effect of an external field, Larmor frequency, absorption process, population of nuclear magnetic energy levels, relaxation processes. Chemical shifts and its measurements. Spin-spin splitting. Rules governing multiplet spectra when $\Delta\upsilon$ / J > 7. Interpretation of NMR spectrum of simple – CH_3OH, C_2H_5OH and $C_6H_5CH_2OH$.

Mass Spectrometry: Principles, Mass spectra- ionization process, molecular ion, base peak. Applications: Identification of compounds from fragmentation patterns. Determination of Molecular formula and Molecular weight – H_2O, CO_2 and $C_2H_5NH_2$.

[15 HOURS]

UNIT-III

ORGANIC CHEMISTRY

Biological Importance of Natural Products: Introduction to Organic Chemistry.

Amino acids, Proteins, carbohydrates (cellulose, starch, glycogen), Lipids (fats and oils, phospholipids), prostaglandins, nucleic acids, terpenoids, steroids, alkaloids, vitamins, flavanoids, natural pigments, flavours (perfumes).

Applications of synthetic products: Dyes, drugs, polymers (plastics) soaps and detergents, insecticides. **[15 HOURS]**

UNIT-IV
PHYSICAL CHEMISTRY

Applications of Physical chemistry: Application of phase rule to two and three component systems. Concepts of entropy and free energy. Partial molar volume and its determination by density measurements. Symmetry elements and symmetry operations, with examples of simple molecules. X-ray diffraction. Bragg equation and Miller indices. Order of a reaction and its determination. Energy of activation and its determination. Assumptions of activated complex theory. Fast reactions with examples. Polymers and their classification. Arrhenius theory of strong and weak electrolytes. Assumptions of Debye-Huckel theory of strong electrolytes. Types of electrodes. Corrosion and its prevention. Laws of photochemistry. Quantum yield and its determination. **[15 HOURS]**

REFERENCES

1. Organic spectroscopy by William Kemp, ELBS Society, MacMillan, 1987.
2. Application of absorption spectroscopy of organic compounds by John R. Dyer, Prentice-Hall of India Private Ltd., New Delhi, 1974.
3. Spectrometric identification of organic compounds, 4th edition, Robert M.Silverstein,
4. G. Clayton Bassler and Terence C. Morrill, John Wiley & Sons Inc., New York, Vol. 1, 1981.
5. Physical Methods for Chemists by R. S. Drago, Saunders College Publishing, NewYork.

6. Quantitative Analysis, R.A. Day and A.L. Underwood, 6th edition, prentice Hall, Inc.1999.
7. Principles of Instrumental Analysis, D.A. Skoog, F.J. Holler and T.A. Nieman, 5th edition, Thomson Asia Pvt. Ltd., Singapore, 1998.
8. Analytical chemistry, G. D. Christian, 5th edition, 2001, John-wiley and Sons Inc. India.
9. Chemical Kinetics by K.J. Laidler.
10. Chemical Kinetics –Moore and Pearson.
11. Kinetics and Mechanism of Chemical Transformation by J. Rajaram and J.C. Kuriacose.
12. Introduction to electrochemistry by S. Glasstone.
13. Thermodynamics for chemists by S. Glasstone, Affiliated East-west press, New Delhi, (1965).
14. Advances in Photochemistry - Rohatgi Mukherjee.
15. Principle and applications of Photochemistry – R.P. Wayne, Elsevier, New York, (1970).
16. Elements of Physical Chemistry – Glasstone and Lewis
17. I. L. Finar, Organic Chemistry, ELBS Longmann, Vol. I & II, 1984.
18. Essentials of physiological chemistry – Anderson, John Wiley & Sons, New York, 1953.
19. K. Albert, L. Lehninger, D. L. Nelson, M. M. Cox, Principles of Biochemistry, CBZ publishers, Ist edition, New Delhi, 1993.
20. Harper's Biochemistry, Ed. R.Harper, 22nd edition, Prentice Hall Press, New York, 1990.
21. Encyclopedia of Chemical technology – Kirck-Othmer series
22. Harper's review of biochemistry – P. W. Martin, P. A. Mayer & V. W. Rodfwell,15th edition, Maurzen Asian Edition, California, 1981.
23. Intrdouction to alkaloids – G. A. Swan.
24. The alkaloids- K. W. Bently.
25. Steroids – L. Fiescher & M. Fiescher.
26. Steroids –Shoppe
27. Inorganic chemistry- J.E.Huheey
28. Chemistry of the elements – Greenwood and Earnshaw.
29. Concise Inorganic chemistry- J.D.Lee.
30. Advanced Inorganic Chemistry – F.A.Cotton and G.Wilkinson
31. Polymer Science – Bill Meyer
32. Symmetry in Molecules – J. M. Hollas
33. Molecular structure – Wheatley
34. X-Ray crystallography - Azaroff

THIRD SEMESTER PRACTICALS

ANALYTICAL CHEMISTRY PRACTICALS

[120 HOURS]

PART-III

1. Determination of calcium in limestone by redox, acid-base and complexation titrations.
1. Determination of calcium in limestone by redox, acid-base and complexation titrations.
2. Determination of aluminium and magnesium in antacids by EDTA titration.
3. Determination of mercury in an algaecide by EDTA titration; and arsenic in ant control preparation by redox titration.
4. Determination of saccharin in tablets by precipitation titration.

5. Electrolytic determination of copper and lead in brass.
6. Polarographic determination of copper and zinc in brass.
7. Determination of sodium, potassium and calcium in mineral waters by atomic emission spectrometry.
8. Determination of iron in mustard seeds and phosphorus in peas by spectrophotometry.
9. Determination of iodine value and saponification value of edible oils.
10. Assay of protein content of wheat flour by kjeldahl method.
11. Determination of ascorbic acid in goose berry/bitter gourd by titrimetry and spectrophotometry.
12. Determination of vitamin A in vanaspathi.
13. Assay of aspirin/caffeine/phenacetin by uv-spectrometry.
14. Determination of sulpha drugs by potentiometry using $NaNO_2$.
15. Analysis of sulphathiazole tablets by non-aqueous titration with tetrabutylammonium hydroxide.
16. Analysis of ephedrine and aspirin tablets by acid-base titration.
17. Analysis of sulphonamides by uv-spectrophotometry.
18. Colorimetric analysis of procaine by diazotization and coupling reaction.
19. Development of a liquid-liquid extraction assay of ephedrine-phenobarbital mixtures.
20. Iodometric determination of pencillin.

PART-IV

1. Anion-exchange separation of chloride and bromide in a mixture**.**
2. Determination of chromium(III) and iron(III) in a mixture by kinetic masking methods.
3. Catalytic determination of traces of selenium in biological materials.
4. Enzymatic determination of glucose in blood.
5. Catalytic determination of iodide in blood serum.
6. Non-aqueous potentiometric titration of a mixture of aniline and ethanol amine.
7. Spectrophotometric determination of lead in waste water using solvent extraction procedure.
8. Thin layer chromatographic separation of amino acids.
9. Qualitative and quantitative analysis of fruit juices for vitamin-C using HPLC.
10. Analysis of brackish water for chloride content by a**)** spectrophotometry (mercuric thiocyanate method) , b) conductometry (silver nitrate) and c**)** potentiometry (silver nitrate)
11. Analysis of a ground water sample for sulphate by titrimetry (EDTA) and turbidimetry.
12. Analysis of a wastewater for total acidity and alkalinity by conductometric titration and comparision with visual methods.
13. Analysis of waste waters for DO and BOD by titrimetry.
14. Determination of fluoride in drinking water/ground water by spectrophotometry (alizarin red lake method).

15. Analysis of waste water for
    a) phosphate by molybdenum blue method
    b) ammonia-nitrogen by Nessler's method
    c) nitrite-nitrogen by NEDA method
16. Determination of soil pH and conductivity.
17. Analysis of a soil sample for
    a) organic carbon by titrimetry and spectrophotometry($K_2Cr_2O_7$ methods)
    b) Calcium carbonate by acid-base titration.
    c) total nitrogen by Kjeldahl method.
    d) calcium and magnesium by EDTA titration.
    e) Available phosphorus by spectrophotometry.
    f) Nitrate-nitrogen/nitrite nitrogen/ammonia nitrogen by spectrophotometry.
    g) sodium and potassium by flame photometry.
19. Analysis of urine for
    h) reducing sugars by titrimetry and spectrophotometry
    i) urea and uric acid by titrimetry and spectrophotometry.
    j) Inorganic phosphorus by spectrophotometry.
    k) Sulphate by precipitation titration after ion-exchange separation.
20. Analysis of blood for
    l) cholesterol by spectrophotometry
    m) urea and uric acid by spectrophotometry
    n) bicarbonate by acid-base titration.

REFERENCES

1. Fundamental of Analytical Chemistry, D.A. Skoog, D.M. West, Holler and Crouch 8th edition, 2005, Saunders College Publishing, New York.
2. Analytical Chemistry, G.D. Christian, 5th ed., 2001 John Wiley & Sons, Inc, India.
3. Quantitative Analysis, R.A. Day and A.L. Underwood, 6th edition,1993 prentice Hall, Inc. New Delhi.
4. Vogel's Textbook of Quantitative Chemical Analysis, J. Mendham, R.C. Denney, J.D. Barnes and M.J.K. Thomas, 6th edition, Third Indian Reprint.2003 Pearson Education Pvt. Ltd., New Delhi.
5. Analytical Chemistry Principles, John H. Kennedy, 2nd edition, Saunders College Publishing, California, 1990.
6. Practical Clinical biochemistry methods and interpretations, R.Chawla, J.P. Bothers Medical Publishers (P) ltd., 1995.
7. Laboratory manual in biochemistry, J. Jayaraman, New Age International Publishers, New Delhi, 1981.
8. Practical clinical Biochemistry-Harold Varley and Arnold.Hein mann, 4th edn.
9. Environmental science: Laboratory Manual, Maurice A. Strabbe, The C.V.Mosbey Co. Saint Loucs, 1972.
10. Experiments on water pollution, D.I.Williams and D. Anglesia, Wayland Publishers Ltd, England, 1978.
11. Experiments on Land pollution D.I.Williams and D. Anglesia, Wayland Publishers Ltd, England, 1978.
12. Experiments in environmental chemistry,P.D.Vowler, and D.W.Counel, Pergamon press, Oxford 1980.

13. Manual soil Laboratory Testing-vol I, K.H. Head, Pentech Press, London 1980.

INORGANIC CHEMISTRY PRACTICALS

[120 HOURS]

PART-III

I. **Analysis of alloys:**

1.Stainless steel

a) nickel gravimetrically using dimethyl glyoxime

b) chromium titrimetrically by persulphate oxidation)

c) iron titrimetrically using cerium sulphate

e) chromium and manganese (simultaneous spectrophotometric method)

2. Ferromanganese: Manganese using EDTA

3.Molybdenum and tungsten steels: gravimetric

4.Wood's alloy:

1.	tin (gravimetric)	
2.	bismuth	titrimetric using EDTA
3.	lead	
4.	cadmium	

II.. Quantitative analysis of the constituents in mixtures containing the following cations:

a. Cu(II) + Fe(II)

Copper – gravimetric as CuSCN

Iron – titrimetric using cerium(IV) solution

b. Cu(II) + Ni(II) –gravimetric using salicylaldoxime.

c. Cr(III) + Fe(III) – using EDTA (Kinetic masking)

III. Semi –micrograviметric estimation of aluminium

IV. Electrogravimetric Estimation of:

i. Copper

ii. Nickel

iii. Copper-nickel alloy

V. Flamephotometric determination of:

iv. Sodium

v. Potassium

vi. Calcium

vii. Lithium

viii. Sodium + Potassium

VI. Polarographic determination of:

a) Cadmium
b) Zinc
c) Cadmium + Zinc

VII. Spectrophotometric determination of the pKa value of an indicator

VIII. Solvent extraction and spectrophotometric determination of:

a. Uranium or molybdenum
b. Nickel

PART-IV

I. Preparation of any FOUR of the following complexes and determination of the purity of the prepared samples and structural study of the prepared complexes using physical methods such as magnetic susceptibility measurements, absorption spectra etc.

a. Chloropentammine cobalt(III) chloride
b. Nitropentaammine cobalt(III) chloride
c. Nitritopentaammine cobalt(III) chloride
d. Hexammine cobalt(III) chloride
e. Mercury tetrathiocyanato cobaltate(II)
f. Hexemine Ni(II) Chloride
g. tris –(thiourea) copper(I) sulphate
h. Potassium tris (oxalato) fernate (III).

II. Stabilization of an unstable oxidation state by complexation: preparation of manganese (III) acetyl acetonate.

III. Preparation of the EDTA complex of Mn(III).

IV. Determination of the composition of a complex of iron-phenanthroline by

a. Job's method
b. Mole-ratio method
c. Slope-ratio method

V. Determination of the stability constant of a complex:

a. Turner –Anderson method (Iron-Tiron OR iron-phenanthroline complex)
b. Bjerrum's method (copper-sulphosalicylic acid)
c. Kinetic method (KI_3 complex)

VI. Preparation and kinetics of the acid hydrolysis of potassium trisoxalato cobaltate(III) trihydrate.

VII. **Demonstration experiments:**

a. Recording and interpretation of IR and NMR spectra of complexes.
b. Interpretation of a simple X-ray powder photograph.
c. TGA of calcium oxalate monohydrate.
d. DTA studies of copper sulphate pentahydrate.
e. Spectrochemical series – evaluation of Dq value.

REFERENCES

1. Advanced physico-chemical experiments – J. Rose.
2. Instrumental analysis manual -Modern Experiments for Laboratory – G.G. Guilbault and L.G. Hargis.
3. A Text Book of quantitative Inorganic Analysis –5th edn. – A.I. Vogel.
4. Experimental Inorganic Chemistry – G. Palmer
5. Inorganic Synthesis – O. Glemser.
6. Experimental Inorganic/Physical Chemistry – Mounir A. Malati.
7. Spectrophotometric determination of elements – Z. Marczenko

ORGANIC CHEMISTRY PRACTICALS

[120 HOURS]

PART-III

1. Fractional crystallization: separation of mixture of naphthalene and biphenyl
2. Fractional distillation: Separation of mixture of benzene and toluene.
3. Thin layer chromatography: Separation of plant pigments
4. Column chromatography: Separation of mixture of o & p-nitro anilines
5. Paper chromatography: Separation of amino acids
6. Isolation of piperine from pepper
7. Isolation of caffeine from tea
8. Isolation of cysteine from hair
9. Isolation of hesperidiene from orange peal
10. Isolation of azeleic acid from castor oil
11. Isolation and spectroscopic characterization of Lycopene

12. Isolation of lipids from egg yolks
13. Extraction of nicotine from Tobacco Leaves

PART-IV

Organic preparations; Multi-step synthesis

1. Oxidation of alcohols: Oxidation of cyclohexanol to adipic acid via cyclohexanone
2. Esterification: Preparation of benzoccaine from p-nitrotoluene
3. Diazotization (Sandmeyer's reaction): Preparation of p-chlorobenzoic acid from p-toluidine
4. Molecular rearrangement:
   i. Preparation of o-chlorobenzoic acid from phthalic anhydride
   ii. Preparation benzillic acid from benzaldehyde
   iii. Preparation of o-hydroxy benzopheneone via Fries rearrangment
   iv. Prepartion of benzanilide from benzophenone oxime.
5. Grignard's reaction: Preparation of triphenyl carbinol
6. Preparation of luminol from phthalic anhydride
7. Preparation of paracetomol.

REFERENCES

1. Manual of Organic Chemistry – Dey and Seetharaman
2. Natural Products Chemistry by Raphel Ikhan
3. Modern experimental organic chemistry by John H. Miller and E. F. Neugil, p 289.
4. An introduction to practical organic chemistry – Robert, Vingrove etc.
5. A Text book of practical organic chemistry – A. I. Vogel Vol. I
6. Practical Organic Chemistry – Mann & Saunders
7. An introduction to practical organic chemistry – Robert, Vingrove etc.
8. Semimicro qualitative organic analysis by Cheronis, Entrikin and Hodnet
9. R. K. Bansal, Laboratory Manual of Organic Chemistry, New PAGE International (P) Ltd. London, 3rd edition, 1996
10. N. K. Visno, Practical Organic Chemistry, New PAGE International (P) Ltd. London, 3rd edition, 1996.

PHYSICAL CHEMISTRY PRACTICALS

[120 HOURS]

PART-III

1. Kinetics of reaction between sodium formate and Iodine, determination of energy of activation and thermodynamic parameters (ΔH, ΔS, ΔG).
2. To study the kinetics of saponification of ethyl acetate by conductivity method, determination of order of reaction w.r.t. [OH^-].
3. To study the kinetics of reaction between acetone and iodine-determination of order of reaction w.r.t. iodine, acetone and H_2SO_4.
4. Conductometric titration of thorium nitrate with potassium tartarate.
5. Determination of mean ionic activity coefficient of a weak electrolyte by conductometric measurements.

6. To study the acid catalysed kinetics of oxidation of glycine by chloramine-T(CAT)-determination of order of reaction w.r.t. [CAT], [glycine] and effect of $[H^+]$.
7. To study the kinetics of autocatalytic reaction between $KMnO_4$ and $C_2H_2O_4$.
8. Kinetics of decomposition of benzene diazonium chloride, determination of energy of activation and thermodynamic parameters.
9. To study the kinetics of solvolysis of t-butyl halide by conductivity method.
10. Potentiometric titration of $Pb(NO_3)_2$ Vs EDTA.
11. Preparation of Ag/AgCl electrode and to determine the activity of 0.2M HCl.
12. Determination of ionic product of water and study the effect of temperature.
13. Determination of transport number by e.m.f. method.
14. Photolysis of monochloro acetic acid.
15. To determine the eutectic point of a two component system (Naphthalene-m-dinitrobenzene, Naphthalene-biphenyl systems).
16. Differential conductometric titration of very weak bases (glycine, p-toluidine, p-phenylenediamine Vs acetic acid or trichloro acetic acid).
17. Conductometric method of determination of solubility of sparingly soluble salt.
18. Potentiometric titration of mixture of KCl+KBr+KI vs $AgNO_3$.
19. Thermodynamic prediction and measurement of solubility of naphthalene in benzene.
20. Study of phase diagram of a three component system (Eg: acetic acid-chloroform-water and benzene-alcohol-water system).
21. Thermodynamics of a cell reaction –construction of an electrochemical cell, study the effect of temperature on the cell reaction and calculation of thermodynamic parameters.

PART-IV

1. Kinetics of decomposition of diacetone alcohol by NaOH-determination of energy of activation and thermodynamic parameters.
2. Spectrophotometric kinetics of oxidation of indigocarmine by chloramine-T(CAT).
    (a) Determination of order of reaction w.r.t. [CAT].
    (b) Effect of pH and determination of order of reaction w.r.t. $[H^+]$.
    (c) Effect of dielectric constant of the medium on the rate of reaction.
3. Kinetic study on Ru(III) –catalysed reaction between primary amine and CAT.
    (a) Determination of order of reaction w.r.t. [amine].
    (b) Determination of order of reaction w.r.t. [Ru(III)].
    (c) Determination of order of reaction w.r.t. $[H^+]$.
    (d) Effect of dielectric constant of the medium (using CH_3OH).
    (e) Determination of Ea and thermodynamic parameters.
4. Kinetics of saponification of ethyl acetate by conductivity method and study the effect of dielectric constant of the medium (using CH_3OH).
5. Study of photolysis of uranyl oxalate: (a) determination of intensity of light source (b) study of photocatalysis of oxalic acid.
6. Photolysis of CAT solution –determinations of quantum yield and study of kinetics of photodecomposition.
7. Preparation of Fricke dosimeter and measurement of the dose rate.
8. Statistical aspects of radioactivity measurements.
9. Determination of maximum beta energy by Nomogram method.
10. Determination of half-life of ^{40}K.

11. Determination of ratio and product of two activities.
12. Potentiometric determination of solubility of sparingly soluble salt (AgCl or $AgBrO_3$). Study of salt effect on solubility and determination of activity coefficient.
13. Differential potentiometric titration of mixture of weak acids (HCOOH, CH_3COOH, $ClCH_2COOH$ Vs NaOH).
14. Determination of pK value of an indicator (methyl orange/bromophenol blue/phenolphthalein etc.).
15. Spectrophotometric analysis of a mixture of (a) $KMnO_4$ and $K_2Cr_2O_7$ (b) $CuSO_4$ and K_2CrO_4.
16. Study of complex formation between ferric salt and salicylic acid.
17. Determination of composition and stability constant of uranyl (V) sulphosalicylate complex by limiting logarithmic method.
18. Determination of half wave potential of metal ions in a mixture (Cd^{2+}, Zn^{2+}, Mn^{2+}, Pb^{2+}, Cu^{2+}).
19. Estimation of a metal ion in solution by polarographic method.
20. Amperometric titration of lead nitrate against potassium chromate/potassium dichromate.
21. Determination of stability constant of lead oxalate complex.
22. Coulometric titrations (a) I_2 Vs $Na_2S_2O_3$ (b) NaOH vs HCl.

REFERENCES

1. Practical Physical Chemistry – A.J. Findlay.
2. Experimental Physical Chemistry –F. Daniels et al.
3. Selected Experiments in Physical Chemistry – Latham.
4. Experiments in Physical Chemistry – James and Prichard.
5. Experiments in Physical Chemistry – Shoemaker.
6. Advanced Physico-Chemical Experiments –J. Rose.
7. Practical Physical Chemistry –S.R. Palit.
8. Experiments in Physical Chemistry – Yadav, Geol Publishing House.
9. Experiments in Physical Chemistry – Palmer.
10. Experiments in Chemistry –D.V. Jahagirdar, Himalaya Publishing House, Bombay, (1994).
11. Experimental Physical Chemistry –Das. R.C. and Behera B, Tata Mc Graw Hill, (1983).
12. .Instrumental Methods in Chemical Analysis, Ewing. G.W, Mc Graw Hill, (1960).
13. Experiments in General Chemistry, CNR Rao and G.C. Agarwal, Affiliated East-West Press, (1966).
14. Polarography – Kolthoff and Lingane.

FOURTH SEMESTER

CH 401 – BIOANALYTICAL CHEMISTRY

[48 HOURS]

UNIT-I

Body fluids: Composition and detection of abnormal level of certain constituents leading to diagnosis, sample collection and preservation of physiological fluids, analytical methods for the constituents of physiological fluids (blood, urine).
Blood: Estimation of glucose, cholesterol, urea, haemeglobin and bilirubin.
Urine: Urea, uric acid, creatinine, calciumphosphate, sodium, potassium and chloride.
Enzymes: Biological significance, analysis and assay of enzymes (pepsin, tyrasinase), vitamins (thiamine ascorbic acid, vitamin A) and harmones (progesterone, oxytocin, insulin), chemical, instrumental and biological assays to be discussed wherever necessary.
Forensic analysis: General discussion of poisons with special reference to mode of action of cyanide organophosphates and snake venom, estimation of poisonous materials such as lead, mercury, and arsenic in biological materials. **[16 HOURS]**

UNIT-II

Pharmaceutical analysis: Importance of quality control, drugs and pharmaceuticals, sources of impurities in pharmaceutical chemicals, analytical quality control in finished/final products common methods of assay.
Analysis of common drugs: Analgesics – aspirin, paracetamol; **Anthelmentics** –mebendazole; **Antiallergies** – chlorpenneramine malleate; **Antibiotics** – pencillin, chloromceytin; **Anti–inflammatory agents** – oxyphenbutazone; **Antimalarials** – primaquine phosphate; **Antituberculosists** – INH; **Narcotics** – nicotine, morphine; **Expectorants** –benadryl; **Sedatives** – diazepam; **Vitamins** – B_1, B_2, B_6 niacin and folic acid. **[16 HOURS]**

UNIT-III

Food Analysis: Historical perspectives, objectives of food analysis. Sampling procedures. Detection and determination of sugars and starch. Methods for protein determination. Oils and fats and their analysis-iodine value, saponification value and acid value. Rancidity-detection and determination (peroxide number). Tests for common edible oils. Analysis of foods for minerals-phosphorus,sodium, potassium and calcium. General methods for the determination of moisture, crude fibre and ash contents of foods. Analysis of milk for fat and added water. Non-alcoholic beverages. Determination of chicory and caffeine in coffee;caffeine and tannin in tea. Alcoholic beverages-methanol in alcoholic drinks and chloral hydrate in toddy. Food additives. Chemical preservatives-inorganic preservatives-sulphur dioxide and sulphites, their detection and determination. Organic preservatives-benzoic acid and benzoates, their detection and determination. Artificial sweetenes-saccharin, cyclamate and dulcin-detection and determination. Flavouring agents-dection and determination of vanilla and vanillin. Coloring matters in foods-classification, certified colours, detection of water soluble dyes, colour in citrus fruits, beet dye in tomato products, mineral colour. Pesticide residues in foods. Determination of chlorinated organic pesticides. **[16 HOURS]**

REFERENCES

1. Pharmaceutical Analysis, T. Higuchi and E.B. Hanssen, John Wiley and Sons, New York.
2. Quantitative Analysis of drugs, P.D. Sethi, 3rd edition, CBS Publishers, New Delhi, 1997.

3. Practical Clinical biochemistry methods and interpretations, R.Chawla, J.P. Bothers Medical Publishers (P) ltd., 1995.
4. Laboratory manual in biochemistry, J. Jayaraman, New Age International Publishers, New Delhi, 1981.
5. Pharmaceutical Analysis, Modern methods-Part A and B, Edited by James W. Munson.
6. Hawk's physiological chemistry-edited by B.L. Oser, 14th edn, Tata Mc Graw Hill.(1976).
7. The Essentials of Forensic Medicine and Toxicology-Dr.K.S. Narayana Reddy.
8. Practical clinical Biochemistry-Harold Varley and Arnold.Hein mann, 4th edn.
9. Analysis of Foods-H.E.Cox.
10. Chemical Analysis of Foods-H.E.Cox and pearson.

CH 402 – BIOINORGANIC CHEMISTRY

[48 HOURS]

UNIT-I

Biochemistry of Sodium, Potassium and Chlorine: Sources, absorption, distribution and functions. The transport mechanism, Na^+, K^+ transporting ATP^{ase} (The Na^+/K^+ pump). Macrocyclic crown ether compounds, cryptands, spherands and ionophores.

Biochemistry of Calcium: Binding, transport and accumulation of Ca^{2+}, calcium and muscle contraction, calcium in blood cloting mechanisms.

Biochemistry of Cobalt: Vitamin B_{12} and B_{12} coenzymes, Coenzyme A, Coenzyme, NAD, FMN and FAD.

Bioenergetics: Energy in biology, energy transfer, the energy of ATP, Kinetic stability of ATP, standard free energy change entropy. High energy compounds, mitochondrial flow of electrons from NADH to O_2.

Bioinorganic Chemistry of Phosphorus: Phosphates and bioenergetics, oxidative phosphorylation-substratate level phosphorylation, respiratory chair phosphorylation, mechanism of oxidative phosphorylation.

Transport and Storage of Iron: Ferretin, transferrin, phosvitin and gastroferrin.

Iron Transport in Microbes: Siderophores, *in vivo* microbial transport of iron.

Bioinorganic chemistry and protection of the environment . **[16 HOURS]**

UNIT –II

Role of metal ions on the catalytic mechanism of enzyme: Ligand bridge complex, metal bridge complex and enzyme bridge complex.

Dioxygen metal complexes in biological system: Reactions of molecular oxygen, activation of dioxygen molecule in transition metal dioxygen complexes.

Oxygen Carrying Proteins: Introduction to porphyrin system, substituent effects on porphyrin rings, hemoglobin and myoglobin, model compounds for oxygen carriers (cobalt, iridium, iron and nickel). Hemerythrin and hemocyanin.

Electron Transport Proteins: Iron-sulphur proteins (rubredoxins and ferredoxins) and cytochromes including cytochrome P450.

Iron and Copper Containing redox enzymes: Catalase and peroxidase. Superoxide dismutase.

Zinc containing enzymes: Alcohol dehydrogenase, carboxypeptidase A.

Molybdenum containing enzymes: Aspects of molybdenum chemistry, xanthine oxidase, aldehyde oxidase, sulphite oxidase, nitrogenase and nitrate reductase. **[16 HOURS]**

UNIT –III

Therapeutic uses of metals and some ligands.
Metal complexes as drugs and therapeutic agents: Introduction, antibacterial agents, antiviral agents, antiarthritis agents and anticancer agents.
Treatment of toxicity due to inorganics: Mechanism of (i) Antidote complexes with poison, rendering it inert (Heavy metals, iron, copper and thallium).
(ii) Antidote accelerated metabolic conversion of poison to non-toxic product (cyanide).
(iii) Antidote cometes with poison for essential receptors (carbon monoxide, morphine and morphine like narcotics). **[16 HOURS]**

REFERENCES

1. Biochemistry – A.L. Lehninger
2. Biochemistry – L. Stryer
3. Bioinorganic Chemistry - R.W. Hay
4. The Inorganic Chemistry of Biological Processes – 2nd edition, M.N. Hughes
5. Bioinorganic Chemistry –M. Satake and Y. Mido.
6. Bioinorganic Chemistry – G.R. Chatwal and Ajaykumar Bhagi.
7. Biological aspects of Inorganic Chemistry – A.W. Addison, W.R. Cullen, D. Dolphin and B.R. James.
8. Principles of drug action: The basis of pharmacology, 2nd edition – A. Goldstein, L. Aronow and S. M. Kalman.
9. Advanced Inorganic Chemistry-II – Gurdeep Raj.
10. Bioinorganic Chemistry.

CH 403 – BIOORGANIC CHEMISTRY

[48 HOURS]

UNIT-I

Amino acids: General structure, physiological properties.
Peptides: Peptide bond, structure determination: C- & N-terminal residue determination, peptide synthesis, Merrifield's solid phase synthesis, selective cleavage of polypeptide bonds (chemical and enzymatic).
Proteins: classification, Isolation and purification; primary, secondary, tertiary and quartenary structure determination, denaturate and renaturing of proteins. , biological application of oxytocin and insulin.
Nucleic acids: Structure and synthesis of nucleosides and nucleotides, structure of RNA and DNA, Crick-Watson model, role of nucleic acids in the biosynthesis of proteins. **[16 HOURS]**

UNIT-II

Carbohydrates: Introduction, Ring size determination of monosaccharides, configuration and conformations of monosachharides, anomeric effect, Hudson's rules, epimerization and mutarotation. Synthesis, industrial and biological importance of glycosides, amino sugars, sucrose, maltose and lactose.
Polysaccharides: General methods of structure elucidation. industrial importance and Biological importance of cellulose, starch, glycogen, dextran, hemicellulose, pectin, agar-agar.Photosynthesis and biosynthesis of carbohydrates. **[16 HOURS]**

UNIT-III

Lipids: Nomenclature, classfication, purification, structure and synthesis of lipids, phospholipids, sphingolipids. Biological importance of lipids :Lecithin, sphingolipids, oils and fats.

Prostaglandins: Introduction, classification and biological importance. Constitution of PGE_1. Synthesis of PGE & F series.

Enzymes: Introduction, nomenclature, classification with examples and their fucntions.

Co-enzymes:

1. Thiamine pyrophosphate (TPP) in oxidative and non-oxidative decarboxylation of α-keto acids and formation of ketols.
2. Pyridoxal phosphate- transamination, decarboxylation, dealdolization and elimination reactions of amino acids.
3. Tetrahydrofolic acid – in one carbon transfer reactions at all oxidation levels except that of CO2.
4. Nicotinamide dinucleotides and flavin coenzymes – in biological oxidation-reduction reactions.

Biosynthesis of fatty acids. **[16 HOURS]**

REFERENCES

1. Essentials of physiological chemistry – Anderson, John Wiley & Sons, New York, 1953.
2. K. Albert, L. Lehninger, D. L. Nelson, M. M. Cox, Principles of Biochemistry, CBZ publishers, ist edition, New Delhi, 1993.
3. Organic Chemistry – Morrison & Boyd
4. I. L. Finar, Organic Chemistry, ELBS Longmann, Vol. I & II, 1984.
5. Harper's Biochemistry, Ed. R.Harper, 22nd edition, Prenctic Hall Press, New York, 1990
6. Encyclopedia of Chemical technology – Kirck-Othmer series
7. Harper's review of biochemistry – P. W. Martin, P. A. Mayer & V. W. Rodfwell, 15th edition, Maurzen Asian Edition, California, 1981.
8. Introduction to the chemistry of fats and fatty acids – F. D. Gunstone.
9. Carbohydrates – Chemistry & Biochemistry –Pigmann & Harton
10. An introduction to carbohydrate chemistry – Guthri & Honeymon

CH 404 – BIOPHYSICAL CHEMISTRY

[48 HOURS]

UNIT-I

Enzyme kinetics: Effect of substrate concentration (Michaelis Menton equation), Effect of pH, effect of catalysts and inhibitors (substrate, zeolite, Cr^{3+}, Fe^{2+} ZnO, U.V light), effect of temperature. A brief kinetic and mechanistic applications of glucose oxidase and L-amino oxidase in the oxidation of glucose and L-amino acids. Biological significance of Donnan membrane phenomenon. Micelles and involvement during digestion and absorption of dietary lipids. Diffusion of solutes across bio-membranes and its application in the mechanism of respiratory Exchange. "Salting In" and "Salting out" of proteins. Osmotic behaviour of cells and osmo-regulation and its application in the evolution of excretory systems of organisms. Effect of temperature and pH on viscosity of Biomolecules (albumin solution). Significance of viscosity in biological systems-mechanism of muscle contraction, detection of intrastrand disulfide bonds in proteins, polymerization of DNA and nature of blood flow through different vessels. Effect of temperature, solute concentration (amino acids) on surface tension. Biological significance of surface tension - stability of Alveoli in lungs, interfacial tension in

living cells (Danielli and Davson model). Application of sedimentation velocity and sedimentation equilibrium method for molecular weight determination of proteins. [16 HOURS]

UNIT-II

Electrokinetic Phenomena: Electrophoresis - principles of free electrophoresis, zone electrophoresis, gel electrophoresis and its applications in qualitative and quantitative study of proteins. Determination of isoelectric point of a protein. Electro osmosis and streaming potential and its biological significan ce.

Pharmocokinetics: Plasma concentration time curve, drug dissolution rate, physico-chemical factors affecting bioavailability. Pharmocokinetics applied to one component open model. Calculation of elimination rate constant and metabolism constant, apparent volume of drug distribution and kinetics of drug clearance. Protein binding of drugs, Bioavailability and bioequivalence. Factors affecting bioavailability, route of drug administration and kinetics of protein binding.

Circular Dicroism (CD) And Optical Rotatory Dispersion (ORD): Principle, Applications- CD/ORD of proteins, CD/ORD of carbohydrates CD/ORD of Nucleic acids and CD of B-DNA and A-DNA. [16 HOURS]

UNIT-III

Homogenous Catalysis: Acid-Base catalysis, specific acid and base catalysis. General acid and base catalysis. Oxidation of amino acids and carbohydrates in pressence of acid and base catalysis.
Acidity functions- Bronstead, Hückel, Hammett and Bunnett hypothesis.

Linear Free Energy Relationship: Hammett equation, Taft equation, Okemoto Brown equation and its application to oxidation of amino acids and aromatic amines. Swain-Scott and Edward equation. Winstein - Grunwald relationship. Isokinetic relationship and significance of isokinetic temperature, Exner criterion.

Kinetic Isotope Effect: Theory of kinetic isotope effect-normal and inverse isotope effect, primary isotope effect, secondary isotope effect, solvent isotope effect. Use of isotopes as tracers in biological study-isotope incorporation and isotope exchange reactions (cleavage of glucose-1-phosphate), In metabolism studies, Radioimmuno assay (labeling of antigens) and Immuno radiometry.

[16 HOURS]

REFERENCES

1. Applied Biopharmoceautics and Pharmacokinetics, Leo Shargel and Andrew Yu, Prentice Hall International, Inc., Fourth Edition.
2. Introduction to Physical Organic Chemistry, R. D. Gilliom, Madison – Wesley, USA (1970).
3. Physical Organic Chemistry, Reaction Rate and Equilibrium Mechanism – L. P. Hammett, McGraw HillBook, Co., (1970)
4. Biophysical Chemistry, Principle and Technique – A. Upadhyay, K. Upadhyay and N. Nath, Himalaya Publishing House, Bombay, (1998).
5. Essentials of Physical Chemistry and Pharmacy – H. J. Arnikar, S. S. Kadam, K. N. Gujan, Orient Longman, Bombay, (1992).

CH 405 –DISSERTATION / PROJECT

[48 HOURS]

CH 406 – (i)- CHEMICAL BIOLOGY

[48 HOURS]

UNIT-I

Life: What is life? Its chemical definition in the perspective of modern scientific progress. **Origin of life**: spontaneous generation of life and its failure; abiotic origin of life : Urey-Miller's experiment, Oparin-Haldane concept of origin of life, panaspermic origin of life and genetic code. life material has come from extra- terrestrial source through meteorites. What is the first important polymer in the evolution of life? RNA based origin of life.

Water – the major constituent of life, its physical and chemical nature that makes it versatile as a solvent. Is life possible without water?.

Cell – the constituent of life: Chemical composition of the cell: brief chemical introduction to the biopolymers like DNA, RNA, protein and polysaccharides; important small molecules like ATP, glucose (their structure and chemistry). Mechanism of organic reactions that are useful in understanding chemical processes inside the cell like addition polymerization with the elimination of water, hydrolysis of ester, Schiffs base formation, decarboxylation reaction, transamination reaction. **[16 HOURS]**

UNIT-II

Basic organic chemistry concepts like nucleophilicity, electrophilicity, different types of addition, substitution and elimination reactions, kinetic isotope effects, proximity effects, stereospecificity and stereoselectivity. Synthetic organic chemistry as employed in biology like formation of new C-C, C-N, C-O bonds etc. Chemical Role of metal ions in the cellular processes (like Mg^{2+}, Ca^{2+}, Fe^{3+}, K^{+} and Na^{+}) [from the perspective of Organic Chemistry]. Molecular enzymology: simple kinetics, enzyme mechanism from the perspective of organic chemistry, allosterism in enzyme mechanism. Chemical basis of the biomolecular recognition: Lock and key hypothesis and Induced Fit theory. Basic non-covalent forces responsible for the specificity in structure and interaction between biomolecules. Brief introduction to chemical thermodynamics and kinetics to understand the chemistry of biological processes with an introduction to different methodologies to study them. Self recognition in biological processes and chemical basis of biological self-assembly with examples of nucleic acid, ribosome and chromatin. Quantitative chemical and physico-chemical approaches to understand biological processes. **[16 HOURS]**

UNIT-III

Modern Techniques in chemical biology: NMR spectroscopy (1,2,3-D), Atomic Force Microscopy, Fluorescence Resonance energy Transfer, Confocal and Fluorescence Correlation Spectroscopy. Drug Discovery: Chemical genomics, basic principles of drug targeting, structure activity relationship, chemical approaches for drug delivery. Chemical Mechanism of drug action – few selective examples of antimicrobial, antiviral and anticancer drugs. System Biology – emerging field to understand the cellular processes. **[16 HOURS]**

REFERENCES

1. Biochemistry - Voet and Voet
2. Molecular Biology of the cell – Alberts et al.

3. Biochemistry - Stryer
4. Organic chemistry – Paula Bruice
5. The Biological Chemistry of the Elements – J. J. R. Frausto da Silva and R. J. P. Williams
6. Foundations of Chemical Biology (Oxford Chemistry Primers) -- C. M. Dobson, J. A. Gerrard, A. J. Pratt
7. Chemical Biology: A Practical Course by Herbert Waldmann

CH 406 – (ii). CHEMISTRY IN INDUSTRY

[48 HOURS]

UNIT-I

Metal Carbides: Salt-like, covalent and interstitial carbides. Intercalation compounds of graphite, alkali metals. Industrially important reactions of oxides with carbon.
Silicone polymers: Introduction, nature of chemical bonds containing silicon, general methods of preparation (fluids and resins) and properties of silicones. Applications. Industrial uses of silicon, silicon carbide and silicon dioxide.
Mica, Clay and zeolites – Structures and applications. Uses of asbestos. Aluminium alloys-Uses.
Chemical reactivity and group trends of germanium, tin and lead – Applications. Metallic tin and alloys, lead alloys and oxides of lead. **[16 HOURS]**

UNIT – II

Industrial production and uses of ammonia and hydrazine. Sulphides and oxoacids of phosphorous. Applications.
Phosphonitrile polymers and phosphazenes.
Nitrides of sulphur: $(SN)_2$ and $(SN)_4$ – preparation, properties, structure and applications.
Sulphides of the metallic elements: General considerations, structural chemistry of metal sulphides, sodium-sulphur batteries and dry batteries. Constituent of paints and types of pigments. TiO_2 as a pigment. Bronze paints.
Ceramics: Raw materials used in ceramics and ceramic insulators. **[16 HOURS]**

UNIT – III

Compounds of arsenic, antimony and Bismuth: Intermetallic compounds and alloys and their uses.
Catalytic applications: Alkene and alkyne complexes. Role of metals in photography and xerography. Monsanto acetic acid process and Monsanto L-Dopa synthesis.
Selected examples of magnetic materials, their structures and properties:
Metals and alloys. Transition metal oxides, spinels, garnets, ilmenites and perovskites. Magnetoplumbites.
Applications: Transformer cores, information storage, permanent magnets.
Solid state layers: The ruby laser and neodymium lasers.. **[16 HOURS]**

REFERENCES

1. Chemistry of the elements – N.N. Greenwood and A. Earnshaw, Pergamon press, 1985
2. Inorganic chemistry – J.E. Huheey.
3. Inorganic polymers – G.R. Chatwal, Himalaya Publishing House, New Delhi.
4. Solid state chemistry and its applications- A.R.West. John Wiley and Sons.

CH 406 – (iii) ENVIRONMENTAL CHEMISTRY

[48 HOURS]

UNIT-I

Air pollution, analysis and control: Historical overview-global implications of air pollution, sources of pollutants, classification of pollutants. Sources and effects of particulates, carbonmonoxide, sulphur oxides, nitrogen oxides, hydrocarbons and photochemical oxidants on human health, vegetation and materials. Standards for air pollutants.

Air quality monitoring: Sampling methods and devices for particulates and gaseous pollutants.SO_2: ambient air measurements and stack gas measurements-Turbidimetric,colorimetric, conductometric and coulometric methods. NO_X: Griess-ilosvay and Jacobs-Hockheiser colorimetric methods, chemiluminiscent technique. CO: NDIR, amperometric, FID and catalytic oxidation methods. Hydrocarbons: total and individual hydrocarbons by gas chromatography. Oxidants and ozone: colorimetric , coulometric, titrimetric,and chemiluminescence methods.

Air Pollution control: Atmospheric cleaning processes, approaches to contaminant control-detection and control at source.

Control devices for particulates: Gravitational settlers, centrifugal collectors, wet collectors, electrostatic precipitation and fabric filtration.

Control devices for gaseous pollutants: adsorption, absorption **,** condensation and combustion processes. Automative emission control-catalytic converters. **[16 HOURS]**

UNIT-II

Water pollution and analysis: Water resources, origin of wastewater, types of water pollutants of their sources and effects, chemical analysis for water pollution control-objectives of analysis, parameters of analysis, sample collection and preservation. Environmental and public health significance and measurement of colour, turbidity, total solids, acidity, alkalinity, hardness, chloride, residual chlorine, chlorine demand, sulphate, fluoride, phosphates, and different forms of nitrogen in natural and waste/polluted waters, heavy metal pollution-public health significance of Pb, Cd, Cr, Hg, As, Cu, Zn and Mn, general survey of the instrumental techniques for the analysis of heavy metals in aquatic systems, organic loadings-significance and measurement of DO, BOD, COD, TOD, and TOC, phenols, pesticides, surfactants and tannin and, lignin as water pollutants and their determination.

[16 HOURS]

UNIT-III

Waste water treatment: Waste water characteristics, effluentstandards, terminology in waste water treatment. Treatment of domestic waste water-preliminary treatment.

Primary treatment: sedimentation, equalization,neutralization.

Secondary treatment: aerated lagoons, trickling filters, activated sludge process, oxidation ditch, oxidation pond and anaerobic digestion. Sludge treatment and disposal.

Tertiary treatment: evaporation, ion-exchange, adsorption, electrodialysis, electrolytic recovery and reverse osmosis.

Advanced waste water treatment: Nutrient removal-nitrogen and phosphorus removal, solids removal.

Waste water disposal and re use. Industrial waste water and its treatment.

Soil Analysis: Inorganic and organic components of soil, collection and preparation of soil samples for analysis. Measurement of soil pH and conductivity. Determination of organic carbon, total nitrogen,

available nitrogen, ammonia nitrogen, nitrate nitrogen and nitrite nitrogen. Available phosphorus and sulphur-their determination. Analysis of soil for sodium, potassium and calcium and magnesium. Micronutrient elements and their analysis. Pesticide residues in soil, their separation and determination. **[16 HOURS]**

REFERENCES

1. Standard Methods of chemical Analysis, A.J.Weleher(part B), Robert E.Kriegor Publishing Co.USA, 1975.
2. Environmental chemistry, S.E. Manahan Willard grant press, London, 1983.
3. Environmental chemical Analysis, Iain L Marr and Malcolm S. Cresser, Blackie and Son, ltd, London, 1983.
4. Chemistry for environmental engineering, Chair N. Sawyer and Perry L. M Canty, Mcgraw Hill Book, Co., Newyork 1975.
5. The Air Pollution Hand Book, Richard Mabey, Penguin, 1978.
6. The pollution Hand Book, Richard Mabey, Ponguin 1978.
7. Soil Chemical Analysis, M.L.Jackson, Prentice Hall of India pvt, ltd., New Delhi,1973.
8. Experiments in environmental chemistry,P.D.Vowler, and D.W.Counel, Pergamon press, Oxford 1980.
9. Manual Soil Laboratory Testing-vol I, K.H. Head, Pentech Press, London 1980.
10. A Text Book of Environmental Chemistry and Pollution Control., S.S. Dara, S.Chand and co. Ltd. New Delhi 2004.
11. Air pollution Vol II edn. by A.C. Stern, Academic Press Newyork, 1968.
12. Instrumental Methods for automatic air monitoring systems in Air Pollution Control, Part-III edn by W.Stranss, John-wiley and sons, New york, 1978.
13. Analysis of Air pollutants, P.O.Warner, John Wiley and sons, New York, 1976.
14. The Chemical Analysis Air pollutants, Interscience, New York, 1960.
15. The Analysis of air pollutants, W.Liethe, Ann Arbor Science Pub.Inc. Michigan 1970.
16. Environmental chemistry, A. K. De.

CH 406 –(iv)- NATURAL PRODUCTS

[48 HOURS]

UNIT-I

Steroids: Introduction, Structure and synthesis of cholesterol. Ergosterol and its irradiation products. Biological importance of bile acids, estrone, progesterone, testosterone, androsterone and corticosterone.

Biosynthesis of cholesterol.

Alkaloids: Introduction, classification, isolation and general methods of structural elucidation. Biological importance of alkaloids. Structure and synthesis of qunine, morphine, reserpine and lysergic acid. Biosynthesis of alkaloids (nicotine and morphine). **[16 HOURS]**

UNIT-II

Vitamins: Introduction, constitution and synthesis of thiamine, riboflavin, pyridoxine, biotin, ascorbic acid, vitamin A, E and K groups. Biosynthesis of vitamin C. **[16 HOURS]**

UNIT-III

Terpenoids: Introduction, classification and general methods of structural elucidation. Biological importance of terpenoids. Chemistry of pinene, camphour, caryophyllene, santonin and squaline.
Porphyrins: Introduction, strucuture and synthesis of haemin. Vitamin B_{12} : structure and as coenzyme in molecular rearrangement reactions; Chlorophyll: structure and biological importance.
Anthocyanins: Introduction, general nature of anthocyanin, Occurrence, structure and synthesis of anthocyanidins, Flavones and isoflavones.
Pheromones: Introduction, classification, source and their use in pest control. Synthesis of disparlure, grandisol, brevicomin and bomykol. **[16 HOURS]**

REFERENCES

1. Organic Chemistry – Morrison & Boyd
2. I. L. Finar, Organic Chemistry, ELBS Longmann, Vol. I & II, 1984.
3. Essentials of physiological chemistry – Anderson, Jhon Wiley & Sons, New York, 1953.
4. K. Albert, L. Lehninger, D. L. Nelson, M. M. Cox, Principles of Biochemistry, CBZ publishers, ist edition, New Delhi, 1993.
5. Harper's Biochemistry, Ed. R.Harper, 22nd edition, Prenctic Hall Press, New York, 1990
6. Encyclopedia of Chemical technology – Kirck-Othmer series
7. Harper's review of biochemistry – P. W. Martin, P. A. Mayer & V. W. Rodfwell, 15th edition, Maurzen Asian Edition, California, 1981.
8. Intrdouction to alkaloids – G. A. Swan
9. The alkaloids- K. W. Bently
10. Steroids – L. Fiescher & M. Fiescher
11. Steroids –Shoppe

CH 406 –(v)- PHARMACOKINETICS

[48 HOURS]

UNIT – I

Rates and order of reactions, Units in Pharmacokinetics, Units for blood concentrations.

Introduction**:** Biopharmaceutics, pharmacokinetics, clinical pharmacokinetics, pharmacodynamics, toxicokinetics and clinical toxicology. Measurement of drug concentration in blood, plasma or serum. Plasma level-time curve, significance of measuring plasma drug concentrations. One compartment open model: Intravenous route of administration of drug, elimination rate constant, apparent volume of distribution and significance. Calculation of elimination rate constant from urinary excretion data, clinical application. Two compartment model: Plasma level-time curve, relationship between tissue and plasma drug concentrations, Apparent volumes of distribution. Drug clearance, clinical example. Plasma level-time curve for a three compartment open model. **[16 HOURS]**

UNIT - II

Drug absorption: Factors affecting the rate of drug absorption-nature of the cell membrane, Route of drug administration- oral drug absorption, Intravenous infusion and intravenous solutions, Effect of food on gastrointestinal drug absorption rate.

Drug Bioavailability: Factors affecting the drug bioavailability, rate of dissolution, pH and drug absorption, particle size, clinical applications. *In vitro – In vivo* correlation of rate of dissolution. Drug release; Kinetics of extended- release dosage forms. Relative and absolute availability, Bioequivalence, clinical significance of bioequivalence studies. Pharmacokinetics of drug absorption, zero-order absorption model, first-order absorption model, determination of absorption rate constant-Waynes-Nelson method, Loo-Reigelman method and its effect on AUC, clinical examples. **[16 HOURS]**

UNIT – III

Kinetics of Protein binding with drugs: Effect of protein binding on the apparent volume of distribution. Determination of binding constants and binding sites by Invitro methods (known protein concentration and unknown protein concentration), Relationship between protein concentration and drug concentration in drug-protein binding. Clinical significance. Kinetics of drug elimination and clearance. Renal drug excretion, relation of rate of drug excretion and drug in the plasma. Kinetics of enzyme inhibition, metabolite pharmacokinetics for drugs in one compartment and two compartment model. Drug biotransformation reaction, effect of blood flow on elimination half-life and hepatic excretion. Non-linear pharmacokinetics, drug elimination by capacity limited pharmacokinetics for one component model (IV Bolus). Determination of Km and Vmax in patients, bioavailibility and protein binding reactions. A brief survey of applications of pharmacokinetics in clinical situations.

[16 HOURS]

REFERENCES

1. Applied Biopharmacokinetics and Pharmacokinetics- Leon Shargel, Andrew Yu Prentice-Hall international, Inc (Fourth edition).
2. Essentials of Physical Chemistry and Pharmacy – H. J. Arnikar, S. S. Kadam, K. N. Gujan, Orient Longman, Bombay, (1992).

CH 406 –(vi)- POLYMER CHEMISTRY

[48 HOURS]

UNIT-I

Basic of Polymers: Importance of polymers. Fundamentals of polymers-Monomers, repeat units, degree of polymerization. Linear, branched and network polymers. Classification of polymers. Polymerization-condensation, addition, free radical, ionic, co-ordination polymerization and ring opening polymerization. Molecular weight and size. Polydispersion. Average molecular weight concepts-number weight and viscosity average molecular weight. Practical significance of molecular weight. Size of polymer molecule.Glass transition temperature Tg – Importance of Tg, factors affecting the temperature. Crystallinity and crystalisability-effect of crystallinity on the properties of polymers. Chemical and Geometrical structures of polymer molecules. Polymer dissolution – criteria for polymer solubility, fractionation of polymers based on solubility. Thermodynamics of polymer solutions. **[16 HOURS]**

UNIT-II

Polymer Characterizations: Isolation and purification of polymers-Fractional precipitation, partial dissolution, gradient elution and Gel permeation chromatography. Principles of determination of molecular weights-End group analysis, viscosity, light scattering, osmometry, cryoscopy, ebulliometry and ultracetrifugation method. Thermal characterization- Isothermal gravimetric analysis,

Thermogravimetry , Differential Thermal Analysis and Differential Scanning Calorimetry. Mechanical properties-Tensile, Impact and Flexural strengths. Flammability and Limiting Oxygen Index. Characterization and structural analysis of polymers - IR, NMR, ESR, X-Ray Diffraction and Scanning Electron Microscopic Methods. **[16 HOURS]**

UNIT-III

Structure Property Relationship: Electrically Conducting polymers – Basics of electrical conduction-Band theory. Structural requirements and factors affecting the conductivity. Design of one – dimesional conducting system. Mechanism of doping. Prospectus of conducting polymers. Applications-light weight rechargeable batteries, solid state batteries and light emitting diodes. Biomedical polymers: Polymers with little contact with blood –contact lenses, dental polymers, adsorbable structures and artificial skin.Materials that are in contact with blood -artificial red blood cells, artificial liver, artificial kidney, artificial lung membranes and artificial heart. Polycarboxylic acid polymers drugs. **[16 HOURS]**

REFERENCES

1. Text book of polymer Science. F.W. Billmeyer, Jr., John Wiley. London (1994).
2. Polymer Science. V. R. Gowrikar, N. V. Vishwanathan and J. Srreedhar, Wiley Eastern, New Delhi (1990).
3. Fundamentals of Polymer Science and Engineering. A. Kumar and S.K. Gupta. Tata –McGraw Hill New Delhi (1978).
4. Polymer Characterization, D. Campbell and J. R. White, Chapman and Hall, New York.
5. Fundamental Principles of Polymer materials, R. L. Rosen, John Wiley and Sons, New York.
6. Infrared spectroscopy by R. T. Conley, Allyn and Bacon, Inc.
7. Functional monomers and polymers by K. Takemoto, Y. Inaki and P. M. Ottenbrite, Marcel dekker, Inc., New York, 1987.
8. Progress in Inorganic Chemistry, by Stephen J. Lippard, John Wiley and Sons, Inc.,New York, vol. **20**, 1976.

CH 406 –(vii)- SOLID STATE CHEMISTRY

[48 HOURS]

UNIT-I

Fundamentals of X-ray crystallography, law of interfacial angles, laws of symmetry, Miller indices, crystal systems, Bravais lattice, X-ray diffraction, Bragg equation, Bragg X-ray spectrometer, Experimental methods – powder and rotating crystal methods, indexing of powder and rotating crystal photographs. Atomic scattering factor, structure factor, Fourier synthesis and electron density diagrams. Electron diffraction of gases, Experimental technique, Scattering-Intensity curves, Wierl equation (no derivation), Radial distribution method, Determination of bond lengths and bond angles.
Imperfections in atomic packings: Types of imperfections. Point defects – Schottky and Frenkel defects. Line defects –dislocation types and dislocation theory. Plane defects and non-stoichiometry. Imperfections and Physical Properties: Electrical, optical, magnetic, thermal and mechanical properties **[16 HOURS]**

UNIT-II

Semiconductors: Band theory, energy bands, intrinsic and extrinsic semiconductors, conductivity: electrons and holes, temperature dependance of conductivity, optical properties: absorption spectrum, photoconductivity, photovoltaic effect and luminescence.
Junction Properties: Metal-metal junctions, metal-semiconductor junctions, p-n junctions, transistors, industrial applications of semiconductors: mixed oxides, spinels and other magnetic materials.
Superconductors: Meissner effect, type I and II super conductors, isotope effect, basic concepts of BCS theory, manifestations of the energy gap, Josephson devices. **[16 HOURS]**

UNIT-III

Chemistry of Nanomaterials : Nano particles. Synthesis-Laser abalation chemical vapour transportor method (CVT) and sol-gel method. Metal oxides nanoparticles with supercritical water and precursor method. Synthesis of metal oxides and its composite nanoparticles by solvothermal and hydrothermal method. Synthesis by micro-oven technique (electromagnetic radiation).Carbon nanotube, Carbon Nanowires and its composites. Magnetic, electrical, electronic and catalytic applications of nanomaterials. Nanomaterials uses in renewable energy. Synthesis of organic nanoparticles (L-Lysine, L-alanine etc). Nano rods-structural and electron transport properties. Inorganic and organic Nano porous Aerogels. Effect of temperature and pH on Nano crystal properties. **[16 HOURS]**

REFERENCES

1. Solid State Chemistry – N.B. Hannay
2. Introduction to solids – Azaroff.
3. Solid State Chemistry and its applications – A.R. West
4. Principles of the Solid State – H.V. Keer.
5. A Text Book of Physical Chemistry – G.M. Barrow. M.C. Graw Hill – Tokyo, (1973).
6. Elements of Physical Chemistry – Lewis and Glasstone.
7. Solid State Chemistry and Its Applications
   Anthony R. West
8. Basic Solid State Chemistry, Second Edition
   Anthony R. West
9. Solid State Chemistry: An Introduction, 3rd edition
   Lesley E. Smart and Elaine A. Moore
10. Introduction to Solid state Physics—C. Kittel, 5th Edition, Wiley Eastern Limited.
11. C.N.R. Rao and J. Gopalakrishna "New Directions in solid state chemistry" Cambridge University Press, Cambridge (1999).
12. Binay Kumar, R.P. Tandon "Advances in technologically important crystals" Macmillan India Ltd.

IN A WEEK, THERE WILL BE TWO HOURS FOR SEMINARS AND ONE HOUR FOR DISSERTATION WORK.

FOURTH SEMESTER PRACTICALS

ANALYTICAL/INORGANIC CHEMISTRY PRACTICALS
ORGANIC/PHYSICAL CHEMISTRY PRACTICALS

[120 HOURS]

Experiments are as in Third semester. Every student will carry out experiments on a rotation basis in the THIRD and FOURTH SEMESTER.