BANGALORE UNIVERSITY

FOR QUALITY & EXCELLENCE
IN HIGHER EDUCATION
A GRADE (3.12)
ACCREDITED BY NAAC

M. Sc., Chemistry (CBCS)

Syllabus

(w. e. f. 2014-2015)

DEPARTMENT OF CHEMISTRY

FOREWORD

As per the directive from the Bangalore University, the syllabus for the M. Sc., Degree course in Chemistry (CBCS) had to be prepared. The Guidelines were provided by the University.

In the Department of Studies in Chemistry, Central College, the Chemistry Teaching Faculty members participated in the syllabus preparation meetings held on 29. 4. 2014, 03. 5. 2014, 10. 5. 2014, 14. 5. 2014 and 26. 5. 2014. Keeping in view the aims of the UGC Model Curriculum in developing interdisciplinary skills in students linking general studies with professional courses and allowing both vertical and horizontal mobility and also catering to local needs. The Teachers of different branches of Chemistry, namely Inorganic, Organic, Physical and Analytical chemistry had separate and joint brainstorming sessions and arrived at a Draft Syllabus in Chemistry for Four semesters M. Sc., course. The Draft Syllabus was then approved by the Department Council in a meeting held on 02. 6. 2014 and finally placed before the Board of Studies in Chemistry (PG) for approval on 11. 6. 2014.

CHAIRMAN
Department of Studies in Chemistry
Central College Campus
Bangalore University
Bangalore-560 001

Proceedings of the meeting of the Board of Studies in Chemistry (PG) held on 11th June 2014 in the Department of Chemistry, Central College Campus, Bangalore University, Bangalore-560001.

A meeting of the Board of Studies in Chemistry (PG) was held on Wednesday the 11th June 2014 at 10.30 am in the Department Library to approve the M. Sc., CBCS syllabus and for the constitution of BOE (PG) in Chemistry and preparation of Panels of Examiners in respect of M. Sc., and Ph. D., viva-voce examinations of 2014-2015.

The Chairman welcomed the members and as per the agenda the M. Sc., CBCS Chemistry syllabus was placed before the members. The Chairman also provided the members with the lists of BOEs constituted for the previous academic years viz, 2011-12, 2012-13 & 2013-14 in respect of the above course and requested the members to constitute the BOE and panel of examiners for the 2014-2015 examinations.

The members after careful scrutiny approved the M. Sc., (CBCS) Chemistry syllabus with modifications wherever necessary, and constituted the BOE (PG) and prepared the panels of examiners in respect of M. Sc., and Ph. D., viva-voce examinations of 2014-2015.

The BOS also ratified the consolidated list of examiners.

The Ph. D., viva-voce panels were approved for the following candidates by the Board members:

1. Ms. Sarika Agarwal
2. Mr. Chilakapati Madhu
3. Mr. M. N. Somashekar
4. Mr. Srinatha, B. S
5. Mr. K. Lokesh

The BOS also made the following recommendations for consideration by the Faculty of Science.

1. It is recommended that the number of contact hours of the Soft Core paper be reduced from the current 3h/week to 2h/week for the purpose of standardization with the hard core papers. Further, the question paper for the soft core paper should be set for a maximum 50 marks (35 paper + 15 IA).
2. It is recommended that a minimum of 8 marks/25 (35%) be specified towards the test component of IA in all the papers, as a qualification for the semester examination.
3. It is recommended that the evaluation of the viva-voce of the Project work/dissertation should be conducted by the Board comprising an internal and one external expert from the panel of examiners and as approved by the Registrar (Evaluation).

Finally the Chairman thanked all the members.

MEMBERS PRESENT

1. Prof. P. Vishnu Kamath

2. Prof. Puttaswamy
3. Prof. Noor Shahina Begum
4. Dr. M. Pandurangappa
5. Dr. V. Gayathri
6. Dr. S. Hari Prasad
7. Prof. S. Anand External Member
8. Prof. J. Keshavayya External Member
9. Prof. M. A. Pasha Chairman (BOS, PG) in Chemistry

SYLLABUS 2014-15

1. Name of the Course : **M.Sc., Chemistry**
2. Duration of the Course : Two Years (FOUR SEMESTERS, CBCS)
3. Eligibility : A candidate must have secured 40% marks in the aggregate and studied Chemistry (cognate subject) securing 50 % marks in this subject at the B Sc., level and studied Mathematics at 10 + 2 or Pre-university level.
4. Intake : 60 + Supernumerary seats + Payment seats
5. Admission : As per University regulations

Scheme of Study and Examination M. Sc., CHEMISTRY

I Semester

Code No.	Title	Theory/ Practical (Hrs/ Week)	Total No.of Hrs/ Semester	Duration of Exam. Hours	Max. Marks (Exam)	Continuous Evaluation	Total Marks	Credits
C-101	Inorganic Chemistry I	4	52	3	70	30	100	4
C-102	Organic Chemistry I	4	52	3	70	30	100	4
C-103	Physical Chemistry I	4	52	3	70	30	100	4
C-104	Biophysical, Bioorganic and Medicinal Chemistry	4	52	3	70	30	100	4
C-105	Green Synthesis (Soft Core)	3	36	3	70	30	100	2
C-105	Photochemistry (Soft Core)	3	36	3	70	30	100	2
C-106	Practical-I Inorg/Org/Phy	4	60	4	35	15	50	2
C-107	Practical-II Inorg/Org/Phy	4	60	4	35	15	50	2
C-108	Practical-III Inorg/Org/Phy	4	60	4	35	15	50	2
C-109	Practical-IV Inorg/Org/Phy	4	60	4	35	15	50	2
	Total marks/credits						**700**	**26**

II Semester

Code No.	Title	Theory/ Practical (Hrs/ Week)	Total No.of Hrs/ Semester	Duration of Exam. Hours	Max. Marks (Exam)	Continuous Evaluation	Total Marks	Credits
C-201	Inorganic Chemistry-II	4	52	3	70	30	100	4
C-202	Organic Chemistry-II	4	52	3	70	30	100	4
C-203	Physical Chemistry-II	4	52	3	70	30	100	4
C-204	Spectroscopy-I	4	52	3	70	30	100	4
C-205	Mathematics for Chemsits (Soft Core)	3	36	3	70	30	100	2
C-206	Practical-I Inorg/Org/Phy	4	60	4	35	15	50	2
C-207	Practical-II Inorg/Org/Phy	4	60	4	35	15	50	2
C-208	Practical-III Inorg/Org/Phy	4	60	4	35	15	50	2
C-209	Practical-IV Inorg/Org/Phy	4	60	4	35	15	50	2
	Total marks/credits						**700**	**26**

Scheme for continuous evaluation

Theory (each paper)
Attendance: 5 marks
Tests* : 25 marks

Total : 30 Marks

* Two tests will be conducted and the average marks of the two tests will be taken for Continuous assessment.

Practicals: (each practical)
Attendance : 3 marks
Records : 2 marks
Tests (2 Tests) : 10 marks

Total : 15 marks

M. Sc., Chemistry III & IV SEMESTERS

(After 2nd semester study tour-cum-industrial visits are proposed in and around Bangalore/Karnataka for the students of 3rd/4th semester)

Scheme of continuous evaluation for all specialisation

Theory (each paper)

Attendance: 5 marks
Tests (2) : 25 marks

Total : **30** Marks

Practicals: (each practical)

Attendance: 2 marks
Records : 3 marks
Tests : 10 marks

Total : **15** marks

M. Sc., Chemistry (Analytical Chemistry Specialisation)
III Semester

Code	**Title of the Paper** ***(Syllabus hours for each theory paper: 52)***	**Teaching/ contact Hrs/week**	**Exam. Hrs.**	**Max. Marks**	**Cont. Eval.**	**Total Marks**	**Credits**
C-301-AC	Principles of Chemical Analysis.	4	3	70	30	100	4
C-302-AC/IC	Advanced Analytical Techniques	4	3	70	30	100	4
C-303-AC/IC/PC	Spectroscopy-II	4	3	70	30	100	4
C-304*	Open Elective	4	3	70	30	100	4
C-305-AC	Analytical (Organic) Practicals- I	4	4	35	15	50	2
C-306-AC	Analytical (Organic) Practicals –II	4	4	35	15	50	2
C307-AC	Analytical Chemistry Practicals- III	4	4	35	15	50	2
C308-AC	Analytical Chemistry Practicals –IV	4	4	35	15	50	2
Total marks/credits						**600**	**24**

* Non-Chemistry Paper

OPEN ELECTIVE FOR NON-CHEMISTRY STUDENTS

Code	**Title of the Paper** ***(Syllabus hours for each theory paper: 52)***	**Teaching/ contact Hrs/week**	**Exam. Hrs.**	**Max. Marks**	**Cont. Eval.**	**Total Marks**	**Credits**
C-304*	Chemistry of Biomolecules (Open Elective)	4	3	70	30	100	4
C-304*	Material Science & Nano materials (Open Elective)	4	3	70	30	100	4

***Number of Students: Min. 10, Max 60.**

M. Sc., Chemistry (Analytical Chemistry Specialisation)
IV Semester

Code	**Title of the paper (*Syllabus hours for each theory paper*: 52)**	**Teaching/ contact Hrs/week**	**Exam Hrs.**	**Max. Marks**	**Continuous Evaluation**	**Total Marks**	**Credits**
C 401-AC	Solid State and Radioanalytical Chemistry	4	3	70	30	100	4
C 402-AC	Environmental & Bioanalytical Chemistry.	4	3	70	30	100	4
C 403-AC/IC	Chemistry of Materials	4	3	70	30	100	4
C 404-AC/IC/PC	Spectroscopy – III	4	3	70	30	100	4
C 405-AC	Analytical practical – V	4	4	35	15	50	2
C 406-AC	Analytical practical –VI	4	4	35	15	50	2
C 407-AC	PROJECT	8		70*	30	100	4
Total marks/credits for the semester						**600**	**24**

* Dissertaion: 50; viv-voce: 20.

M. Sc. Chemistry (Inorganic Specialisation)
III Semester

Code	**Title of the Paper** ***(Syllabus hours for each theory paper: 52)***	**Teaching /contact hrs/week**	**Examination Hrs.**	**Max. Marks**	**Cont. Eval.**	**Total Marks**	**Credits**
C-301-IC	Solid State Chemistry	4	3	70	30	100	4
C-302-AC/IC	Advanced Analytical Techniques	4	3	70	30	100	4
C-303 AC/IC/PC	Spectroscopy-II	4	3	70	30	100	4
C-304*	Open Elective	4	3	70	30	100	4
C-305-IC	Inorganic Chemistry Practicals-I	4	4	35	15	50	2
C-306-IC	Inorganic Chemistry Practicals-II	4	4	35	15	50	2
C307-IC	Inorganic Chemistry Practicals-III	4	4	35	15	50	2
C308-IC	Inorganic Chemistry Practicals-IV	4	4	35	15	50	2
Total marks/credits for the semester						**600**	**24**

* Non-Chemistry Paper

M. Sc. Chemistry (Inorganic Specialisation)
IV Semester

Code	**Title of the paper (Syllabus hours for each theory paper:52)**	**Teaching/ contact hrs/week**	**Exam Hrs.**	**Max. Marks**	**Continuous Evaluation**	**Total Marks**	**Credits**
C 401-IC	Organometallic Chemistry & Catalysis	4	3	70	30	100	4
C 402-IC	Inorganic Recation Mechanisms & Bioinorganic Chemistry	4	3	70	30	100	4
C 403-AC/IC	Chemistry of Materials	4	3	70	30	100	4
C 404-AC/IC/PC	Spectroscopy – III	4	3	70	30	100	4
C 405-IC	Inorganic practical – V	4	4	35	15	50	2
C 406-IC	Inorganic practical – VI	4	4	35	15	50	2
C 407-IC	PROJECT	8		70*	30	100	4
Total marks/credits for the semester						**600**	**24**

* Dissertaion: 50; viv-voce: 20.

M. Sc., Chemistry (Organic Specialisation)

III Semester

Code	**Title of the Paper** ***(Syllabus hours for each theory paper: 52)***	**Teaching/ contact hrs/week**	**Examination Hrs.**	**Max. Marks**	**Continuous Evaluation**	**Total Marks**	**Credits**
C-301-OC	Organic Reaction Mechanisms	4	3	70	30	100	4
C-302-OC	Chemistry of Natural Products	4	3	70	30	100	4
C-303-OC	Organic Spectroscopy	4	3	70	30	100	4
C-304*	Open Elective	4	3	70	30	100	4
C-305-OC	Organic Chemistry Practicals-I	4	4	35	15	50	2
C-306-OC	Organic Chemistry Practicals-II	4	4	35	15	50	2
C307-OC	Organic Chemistry Practicals-III	4	4	35	15	50	2
C308-OC	Organic Chemistry Practicals-IV	4	4	35	15	50	2
Total marks/credits for the semester						**600**	**24**

* Non-Chemistry Paper

M. Sc., Chemistry (Organic Specialisation)

IV Semester

Code	**Title of the paper (Syllabus hours for each theory paper:52)**	**Teaching/ contact hrs/week**	**Exam Hrs.**	**Max. Marks**	**Continuous Evaluation**	**Total Marks**	**Credits**
C-401-OC	Organometallic and Heterocyclic Chemistry	4	3	70	30	100	4
C-402-OC	Stereochemistry & Retrosynthetic Analysis	4	3	70	30	100	4
C-403-OC	Organic Synthesis	4	3	70	30	100	4
C-404-OC	Medicinal Organic Chemistry	4	3	70	30	100	4
C-405-OC	Organic Chemistry Practical-V	4	4	35	15	50	2
C-406-OC	Organic Chemistry Practical-VI	4	4	35	15	50	2
C 407-OC	PROJECT	8		70*	30	100	4
Total marks/credits for the semester						**600**	**24**

* Dissertaion: 50; viv-voce: 20.

M.Sc. Chemistry (Physical Specialisation)

III Semester

Code	**Title of the Paper** ***(Syllabus hours for each theory paper: 52)***	**Teaching /contact hrs/week**	**Examination Hrs.**	**Max. Marks**	**Continuous Evaluation**	**Total Marks**	**Credits**
C-301-PC	Solid State Chemistry	4	3	70	30	100	4
C-302-PC	Surface & Quantam Chemsitry	4	3	70	30	100	4
C-303-AC/IC/PC	Spectroscopy-II	4	3	70	30	100	4
C-304*	Open Elective	4	3	70	30	100	4
C-305-PC	Physical Chemistry Practicals-I	4	4	35	15	50	2
C-306-PC	Physical Chemistry Practicals-II	4	4	35	15	50	2
C307-PC	Physical Chemistry Practicals-III	4	4	35	15	50	2
C308-PC	Physical Chemistry Practicals-IV	4	4	35	15	50	2
Total marks/credits for the semester						**600**	**24**

* Non-Chemistry Paper

M.Sc. Chemistry (Physical Specialisation)

IV Semester

Code	**Title of the paper (Syllabus hours for each theory paper: 52)**	**Teaching / contact hrs/week**	**Exam Hrs.**	**Max. Marks**	**Continuous Evaluation**	**Total Marks**	**Credits**
C-401-PC	Applied Electrochemistry	4	3	70	30	100	4
C-402-PC	Physical Chemistry of Macromolecules	4	3	70	30	100	4
C-403-PC	Kinetics and Reaction Mechanism	4	3	70	30	100	4
C 404-AC/IC/PC	Spectroscopy – III	4	3	70	30	100	4
C-405-PC	Physical Chemistry Practicals-V	4	4	35	15	50	2
C-406-PC	Physical Chemistry Practicals-VI	4	4	35	15	50	2
C 407-PC	PROJECT	8		70*	30	100	4
Total marks/credits for the semester						**600**	**24**

* Dissertaion: 50; viv-voce: 20.

FIRST SEMESTER

C-101 INORGANIC CHEMISTRY – I

52 Hours

UNIT- I

Chemical Bonding- VSEPR model, shapes of molecules-ClF_3, ICl_4^-, TeF_5^-, I_3^-, $TeCl_6^{2-}$, XeF_6, $SbCl_6^{3-}$, IF_7, ReF_7, XeF_8^{2-}, TaF_8^{3-}; Bent rules and energetics of hybridization; electronegativity and partial ionic character; Bonds- Multicenter, Synergic and Agostic bonding.
Lattice energy: Born-Lande equation, Kapustinskii equation; polarizability and partial covalent character, radius-ratio rules, structures of simple solids, Zintl- isoelectronic relationship in solids.
Molecular orbital theory: LCAO and MO diagrams of heteronuclear diatomic (CO, NO, HF, ICl) and triatomic molecules (CO_2 and NO_2^-). **13h**

UNIT- II

Chemistry of main group elements- Structure and bonding in boranes, carboranes, metallocarboranes, Wades rules, borazines, phosphazenes, S,N- compounds.
Silicates- Classification, structures, isomorphous replacement, pyroxenes, layered and vitreous silicates, zeolites and molecular sieves. **13h**

UNIT-III

HSAB concept: Basis of HSAB concept, acid-base strength, hardness and softness, symbiosis, applications of HSAB concept; Acid- base concept in non-aqueous media, reactions in BrF_3, N_2O_4, anhydrous H_2SO_4, CH_3COOH.
Isopoly and heteropoly acids of W, Mo and V, preparations, properties, structure and applications.
Stereoisomerism- Chirality, optical activity- CD, ORD, Cotton effect, absolute configuration of metal complexes, magnetic circular dichroism. **13h**

UNIT-IV

A. M-M bond and metal atom clusters, halide clusters, bonding in $[ReCl_8]^{2-}$. Metal carbonyl clusters- LNCC's and HNCC's. Electron counting in carbonyl clusters, Wades-Mingos and Lauher rules.
B. Nuclear Chemistry-The atomic nucleus-elementary particles, quarks, classification of nuclides based on Z and N values, nuclear stability, nuclear potential, binding energy. Nuclear Models: Shell model-salient features, forms of the nuclear potential, filling of orbitals, nuclear configuration, Liquid drop model, Fermi gas model, Collective model and Optical model. Radioactivity, radioactive decay kinetics, Parent-daughter decay-growth relationship-secular and transient equilibria, theories of α, β^-, β^+ and γ-decay, internal conversion, Auger effect.

13h

SUGGESTED BOOKS

1. Basic Inorganic Chemistry- F. A. Cotton, G. Wilkinson and P. L. Gaus; John Wiley and sons. Inc, 6th edition (1999).
2. Advanced Inorganic Chemistry, 6th edition; F. A. Cotton and G. Wilkinson.
3. Inorganic Chemistry IV edition; J. E. Huheey, E. A. Keiter and R. L. Keiter, Addison; Wesley (1993).
4. Inorganic Chemistry, II edition, D. F. Shriver, P. W. Atkins and C. H. Langford, ELBS; Oxford University Press, 1994.
5. Chemistry of elements; N. N. Greenwood and A. E. Earnshaw, Butterworth Heinemann (1997).
6. Concise Inorganic Chemistry, 5th edition; J. D. Lee (1996).
7. Essentials of nuclear chemistry, 4th edition; H. J. Arniker, NAIL publishers (1995); Chapters 1, 3 and 4.
8. Nuclear and Radioactive chemistry; Friedlander, Kennedy and Miller; Chapters 8 and 9.
9. Inorganic Chemistry, 3rd Edition; Gary. L. Miessler and Donald . A. Tarr (2007).

C-102: ORGANIC CHEMISTRY- I

52 Hours

UNIT-I

Nature of Bonding in Organic Molecules **6h**

Delocalized chemical bonding: Conjugation, cross conjugation, resonance.
Aromaticity. Huckel's rule of aromaticity.Aromatic systems with electron numbers other than six (including azulene, tropone, tropolone and annulenes). Antiaromaticity. Aromaticity in benzenoids, meso-ionic compounds. Homo-aromaticity. Alternant and nonalternant hydrocarbons, Energy levels in odd and even-alternant hydrocarbons, energy levels for the benzyl cation, benzyl free-radical and benzyl carbanion. Hyperconjugation. Tautomerism.

Reaction Mechanisms-I **7h**

Generation, structure, stability and reactivity of carbocations, carbanions, carbon free radicals, carbenes and nitrenes.
Classification of reactions and mechanisms. Thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammond postulate, Curtin-Hammett principle. Potential energy diagrams, transition states and intermediates.
Methods of determining mechanisms: Based on the structure of products, determination of the presence of intermediates, isotopic labeling, isotope effects, from stereochemical evidence.
Acids and bases: Hard and soft acids and bases. Effect of structure on the strengths of acids and bases.

UNIT-II

Reaction Mechanisms-II **5h**

Effect of structure on reactivity:- Resonance and field effects; steric effects. The Hammett equation and linear free energy relationship, substituent and reaction constants. Taft equation.
Nucleophilic substitution reaction at a saturated carbon: SN1, SN2, and SET mechanisms. Effect of substrate structure, attacking nucleophile, leaving group.Ambident nucleophiles and substrates.

Stereochemistry-I **8h**

Fischer, Newman, Sawhorse and flying wedge projections and their interconversions.Optical isomerism: Elements of symmetry and chirality. D-L conventions. CIP rules,
R-S and M-P conventions.Chirality in compounds with a stereogenic centre, and in allenes, alkylidene cycloalkanes and spiranes (with a stereogenic axis).
Cram's and Prelog's rules.
Conformational analysis: Conformational analysis of cycloalkanes: cyclobutane, cyclopentane, cychexanes (monosubstituted e.g., methyl, *iso*-propyl, *tert*-butyl and di-substituted cyclohexanes e.g., dialkyl, dihalo, diols), and cycloheptane.

UNIT-III

Stereochemistry-II **2h**

Nomenclature and conformations of fused rings and bridged ring systems.
Prochirality: Enantiotopic and diastereotopic atoms, groups and faces.

Carbohydrates **9h**

Introduction. Kiliani-Fischer synthesis, Determination of configuration of the monosaccharides, conformational analysis of monosaccharides. Synthesis of amino sugars (β-D- Glucosamine, galactosamine, N-acetylmuramic acid (NAMA), N-acetyl neuraminic acidNANA). C- and N-glycosides. Synthesis of aldonic, uronic, aldaric acids and alditols.Structure elucidation of sucrose and maltose.Structures of lactose, gentiobiose, and meliobiose.Photosynthesis of carbohydrates.

UNIT-IV

Heterocyclic compounds **8h**

Nomenclature of heterocyclic compounds.

Structure, reactivity, synthesis and reactions of pyrazole, imidazole, oxazole, isoxazole, thiazole, isothiazole, pyrimidine, purine and indole. Preparation and reactions of coumarins, acridines, cinnolenes and quinoxalines.

Vitamins **7h**

Biological importance and synthesis of Vitamins A, Vitamin B_1 (thiamine), Vitamin B_6 (pyridoxine), folic acid, pantothenic acid, riboflavin, Vitamin C, Vitamin E (α-tocopherol), Vitamin H (biotin), Vitamins K_1 and K_2.

SUGGESTED BOOKS

1. Advanced Organic Chemistry – Reactions, Mechanism and Structure, Jerry March, John Wiley (2008).
2. Advanced Organic Chemistry, F A Carey and R J Sundberg Plenum, (1990).
3. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman, (2000).
4. Structure and mechanism of Organic Chemistry, C K Ingold, Cornell University Press (1999).
5. Organic Chemistry, R T Morrison and R N Boyd, Prentice-Hall, (1998).
6. Modern Organic Reactions, H O House, Benjamin, (1972).
7. Principles of Organic Synthesis, R O C Norman and J M Coxon, Blackie Academic and Professional, (1996).
8. Stereochemistry of Organic Compounds, D Nasipuri, New-Age International, (1999).
9. Stereochemistry of Carbon Compounds, E L Eliel, S H Wilen and L N Mander, John Wiley, (1994).
10. Stereochemistry, Potapov, MIR, Moscow, 1984.
11. Organic Chemistry, Volumes I and II, I L Finar, Longman, (1999).

C-103: PHYSICAL CHEMISTRY- I

52 Hours

UNIT-I

Quantum Mechanics-I **13h**

Introduction to quantum mechanics. Schrödinger wave equation. Time-independent and time-dependent Schrödinger wave equations and the relation between their solutions. Eigenfunctions and Eigenvalues. Physical Interpretation of wave function. Concepts of Operators: Laplacian, Hamiltonian, Linear and Hermition operators. Angular Momentum operators and their properties. Commutation of operators. Normalization, orthogonality and orthonormality of wave functions. Average (expectation) values. Postulates of quantum mechanics. Solutions of Schrödinger wave equation for a free particle, particle in a ring, particle in a three dimensional box. Quantum mechanical degeneracy, tunneling (no derivation). Application of Schrödinger equation to harmonic oscillator, rigid rotator. Eigenfunctions and eigenvalues of angular momentum. Ladder operator method for angular momentum.

UNIT-II

Quantum Mechanics-II **13h**

Schrödinger equation to hydrogen atom in spherical polar co-ordinates. Solution of Φ, Θ, equation and statements of solution of R equation. Total wave functions of hydrogen atom. Quantum numbers and their characteristics. List of wave functions for few initial states of hydrogen like atoms. Diagrams of radial and angular wave functions. Radial and angular distribution function and their significance. Electron spin (Stern-Gerlach experiment), spin-orbital, anti-symmetry and Pauli-exclusion principle, Slater determinants. Coupling of Angular momenta. Russell-Saunders and JJ-coupling, Term symbols. Spin-orbital interaction and explanation of term multiplicities (Na-D doublet). Zeeman effect.
Approximate methods: Need for approximate methods. Perturbation method. Rayleigh Schrödinger perturbation theory for time-independent non-degenerate system. Application to electron in a box under the influence of an electric field. Application to He atom. Variation theory-statement and proof. Application of variation method to particle in a one-dimensional box and He atom.

UNIT-III

Chemcal Dynamics-I **13h**

A. Macroscopic and microscopic kinetics, Review of theories of reaction rate-Collision theory and Transition state theory, Comparison of collision theory with transition state theory, Arrhenious equation- characteristics, Significance of energy of activation, Temperature coefficient and its evaluation. Thermodynamical formulation of reaction rates (Wyne-jones and Eyring treatment), Reaction between ions in solutions – Influence of ionic strength on reaction rates (primary and secondary salt effects). 5h

B. Concept of Steady state kinetics, Chain reactions – chain length and chain inhibition, comparison of photochemical and thermal reactions, Mechanisms of thermal and photochemical reactions between hydrogen-bromine and hydrogen-chlorine. Comparative study of thermal and photochemical hydrogen-halogen reactions. Pyrolysis of acetaldehyde, Decomposition of ethane. 4h

C. Kinetics of fast reactions- Introduction, Study of reactions by relaxation method (Temperature and pressure jump), flow method (Plug flow method and Stopped flow method), Flash photolysis and Shock tube method. 4h

UNIT-IV

Chemcal Dynamics-II **13h**

D. Kinetics of homogeneous catalysis-kinetics of auto catalytic reactions, kinetics of acid-base catalysed reactions. Comparison of enzyme catalysed and chemical catalysed reactions, Mechanism (Lock and Key theory), Kinetics of enzyme catalyzed reactions – Henri-Michaelis-Menten mechanism, Significance of Michaelis-Menten constant, Lineweaver-Burk plot. Effects of enzyme concentration, pH, Temperature, Activators and Inhibitors on enzyme activity. 5h

E. Theories of unimoleuclar reactions: Perrin theory, Lindemann theory, and Hinshelwood theory. 3h

F. Surface chemistry- Types of adsorption isotherms, Effect of temperature on adsorption, Mechanical adsorption, Estimation of surface area using BET equation, Gibbs adsorption isotherm and its significance, Surface tension and surface energy, Pressure difference across curved surface (Laplace equation), Vapour pressure of droplets (Kelvin equation), Surface film on liquids (electro-kinetic phenomena), Catalytic activity of surfaces. 5h

SUGGGESTED BOOKS

1. Physical Chemistry, P. W. Atkins, Julio de Paula, ELBS, 7th edition, (2002).
2. Physical Chemistry: A Molecular Approach, McQuarie and Simon, Viva, New Delhi, (2001).
3. Introduction to Quantum Chemistry, A. K. Chandra, Tata McGraw Hill, (1988).
4. Quantum Chemistry, Ira. N. Levine, Prentice Hall, New Jersey, (1991).
5. Quantum Chemistry, R. K. Prasad, New Age International, 2nd edition, (2000).
6. Quantum Chemistry through problems and solutions, R. K. Prasad, New Age International (1997).
7. Chemical Kinetics- K. J. Laidler, McGraw Hill. Inc. New York (1988).
8. Principles of Chemical Kinetics – House J. E. Wm C Brown Publisher, Boston, (1997).
9. Kinetics and Mechanism – A. A. Frost and R. G. Pearson, John-Wiley, New York, (1961).
10. Chemical Kinetic Methods – C. Kalidas, New Age International Publisher, New Delhi (1995)
11. S.H. Maran and C. F. Pruton, 4th Edn., Oxford, & IBH publishing Co. Pvt. Ltd. New Delhi (1965).
12. Physical Chemistry- P. Atkins and J. D. Paula, 9th Edn., Oxford University Press (2010).
13. Biochemistry, - Geoffrey Zubay, 2nd Edn.,Macmillan Publishing Co. New York (1981).
14. Kinetics and Mechanism of Chemical Transformations- J. Rajaraman and J. Kuriakose, Mc Millan. (1986).
15. Physical Chemistry of Surfaces- A. W. Adamson, Interscience Publisher Inc., New York (1967).
16. Surface Chemistry: Theory and Applications, J. J. Bikerman, Academic Press. New York (1972).

C-104: BIOPHYSICAL, BIOORGANIC AND MEDICINAL CHEMISTRY

52 Hours

PART A: BIOPHYSICAL CHEMISTRY

UNIT-I

13h

BIOENERGETICS

Standard free energy, entropy and chemical potential change in biochemical reactions.The effect of temperature and pH on ΔG^o.Methods of determination of free energy changes.Relationship between K_{eq} and ΔG^o.Oxidation, reduction reaction and hydrolytic reactions in biological system, redox potential (electron-transfer reactions), free energy changes of oxidation-reduction reactions. Problems solving.

PROPERTIES OF WATER

Ionic product of water and its measurements.Importance of water in biological system with special reference to the maintenance of the native structure of biological molecules.Types of bonding in biological molecules.Biological relevance of pH and pK_a of functional groups in biopolymers, proteins and nucleicacids. Buffers,pH value of various bio-entities, buffer action, buffer capacity and their importance in biological systems. Isoelectric points for amino acids.Titration of proteins and preparation of buffer. Problem solving.

UNIT-II

13h

BIOPOLYMER INTERACTIONS

Forces involved in biopolymer interaction. Electrostatic charges and molecular expansion, hydrophobic forces, dispersion force interaction. Multipleequilibria and various types of binding processes in biological system.Hydrogen ion titration curve.Thermodynamics of biopolymers.Vant's Hoff's law of osmotic pressure, Theory of osmotic pressure and semipermiability.Behaviour of cells and molecular weight determination from osmotic pressure measurements. Significance of osmosis in biology. Problem solving.

TRANSPORT OF IONS

Ion transport through cell membrane, irreversible thermodynamic treatment of membrane transport.

BIOSENSORS

Definition, types, sensors for environmental, medical, food safety and biosecurity applications.

PART B: BIOORGANIC AND MEDICINAL CHEMISTRY

UNIT-III

13h

Synthetic Molecular Receptors: Definition and Significance. Structure and function of receptors with molecular clefts, molecular tweezers, Receptors with multiple hydrogen bonding sites, Crown ether, Cryptates; Cyclodextrins, Cyclophanes, Calixarenes, ionophores, and micelles.

Fatty acid metabolism: Biological importance of factty acids and lipids, even chain and odd chain fatty acids, saturated and unsaturated fats, ketone bodies, fatty acid metabolism, calorific value of foods, biological membranes, properties and function of lipid bilayers and liposomes. Biosynthesis of lipids, amino acids and carbohydrates.

UNIT-IV

13h

Concepts of Medicinal Chemistry: Important terminology in medicinal Chemistry, Drug, Pharmacy, Pharmaceutics, Toxicology, Pharmacodynamics agents, Pharmacophore, pharmacodynamics, metabolites and anti-metabolites, chemotherapy.
Mechanism of chemotherapeutic actions: 1) Biological defences. 2) Chemical defences. a) Surface active agents; b) Metabolic antagonism. Assay of Drugs: Chemical Assay, Biological Assay, Immunological Assay, LD_{50}, ED_{50}, IC_{50} and ID_{50}.

Classification and nomenclature of Drugs

i) Classification of drugs on the basis of therapeutic action.
ii) Nomenclature of Drugs.
iii) Difference Drugs and medicines.

Drug Discovery

i) Introduction
ii) Procedure followed in Drug Design. a) Drug Discovery without a lead b) Lead Discovery.
iii) Lead Modification: Drug Design and Development
iv) Identification of active part: The pharmacophore b) Functional group modification, c) Structure-activity relationship d) Structure modification to increase potency and the therapeutic index: 1. Homologation; 2. Chain branching; 3. Ring-chain transformation; 4. Bioisosterism Structural Modification to increase oral Bioactivity.
    1) Electronic Effect; 2) The Hammet equation; 3) Lipophilicity effect.

Concept of Prodrugs and soft drugs.

a) Prodrugs: i) Prodrugs designing, types of prodrugs; ii) Prodrug formation of compounds containing various chemical groups, Prodrugs and Drug delivery system
b) Soft drugs: i) soft drug cocept; ii) Properties of soft drugs.

SUGGESTED BOOKS

Part A: Biophysical Chemistry

1. Chemistry – An introduction to general, organic and biological chemistry, VII Edn ,Karen C Timberlake, Benjamin/ Cummings, 1999.
2. Biological Chemistry by James P Allen, Wiley-Blackwell, 2008.
3. Biochemistry: Rawn, J. David, N. Patterson Publishers, 1989.
4. Introduction to Biophysical chemistry, R. Bruce Martin, McGraw-Hill, NY, 1964.
5. Physical Chemistry with applications to Biological systems, Ramond Chnag, Mc Millan publishing Co.inc, New York 1977.
6. Macromolecules: Structure and function, F. Wold, Prentice Hall, 1972.
7. Physicalbiochemistry; applications to biochemistry and molecular biology by Freifelder, David, San Francisco; WH Freeman and Company; 1976.

8. Environmental Biosensors, Edited by Vernon Somerset, ISBN 978-953-307-486-3, 356 pages, Publisher: InTech, Chapters, published under CC BY-NC-SA 3.0 license DOI:10.5772/929, 2011.

Part B: Bioorganic and Medicinal Chemistry

1. Gringauz, A. Introduction to Medicinal Chemistry: How Drugs Act and Why? John Wiley & Sons (1997).
2. Dugas, H. & Penny, C. Bioorganic Chemistry: A Chemical Approach to Enzyme Action, Springer Verlag (1998).
3. Bioorganic, Bioinorganic and Supramolecular Chemistry, P. S. Kalsi and J. P. Kalsi. New Age International Publishers.
4. The Organic Chemistry of Biological Pathways By John McMurry, Tadhg Begley by Robert and company publishers.
5. Biochemistry By Lehninger
6. Natural products Chemistry and applications, Sujata V Bhat, B. A. Nagasampagi and S. Meenakshi, Narosa Publishing House.
7. L. Stryer, Biochemistry, 5th edition (2002), Freeman & Co., New York.
8. D. L. Nelson and M.M. Cox, Lehninger Principles of Biochemistry, 3rd edition (2002) McMillan North Publication.
9. The Organic Chemistry of Drug Design and Drug Action. by R.B. Silverman, Academic Press,1992.
10. Drug Designs- A series of monographs in medicinal chemistry edited by A.J. Ariens. Ist edition. Vol. I, II, V, VIII & IX (only relevant chapters).
11. Comprehensive medicinal chemistry. Peragmon Press. 1990, Vol.4.
12. Burger's Medicinal Chemistry & Drug Discovery .fifth edition vol-.I, Willey Interscience.

C-105 GREEN SYNTHESIS (SOFT CORE)

36 Hours

UNIT-I

Use of ultrasound and Microwaves in Organic Synthesis **8h**

Use of ultrasound**:** Introduction, instrumentation, the phenomenon of cavitation. Sonochemical esterification, substitution, addition, alkylation, oxidation, reduction and coupling reactions.

Use of Microwaves: Introduction, concept, reaction vessel/medium, specific effects, atom efficiency (% atom utilization), advantages and limitations. N-alkylation and alkylation of active methylene compounds, condensation of active methylene compounds with aldehydes and amines. Diels-Alder reaction. Deprotection of esters and silyl ethers. Oxidation of alcohols and sulfides.

UNIT-II

Ionic-liquids: Introduction, structure, synthesis and applications of some important ionic liquids in organic synthesis. . **3h**

Polymer supported reagents in organic synthesis

Introduction- properties of polymer support, advantages of polymer supported reagents and choice of polymers.

Applications: Substrate covalently bound to the support: Synthesis of oligosachcharides, Dieckmann cyclisation. Preparation of polymer bound aldehyde and application in aldol and Wittig reactions. Synthesis of polystyryl boronic acid and use in diol protection reaction.

Reagent linked to a polymeric material: Preparation of sulfonazide polymer and application in diazotransfer reaction. Synthesis of polymer bound per acid and its applications.

Polymer supported catalytic reactions: Preparation of polymer supported $AlCl_3$ and application in etherification and acetal formation reactions. **8h**

UNIT-III

Phase transfer catalysis and Crown ethers **8h**

Phase transfer catalysis: Introduction, definition, mechanism of phase transfer catalysis. Types of phase transfer catalysts and reactions and their Advantages.

Preparation of catalysts and their application in substitution, elimination, addition, alkylation, oxidation and reduction reactions.

Crown ethers: Introduction, nomenclature, features, nature of donor site. General synthesis of Crown ethers.

Synthetic applications: Alkylation, generation of carbenes, aromatic substitution and displacement reactions. Generation and application of superoxide anions. Cation deactivation reactions.

UNIT-IV

Multi-component Reactions **9h**

Studies on the mechanistic aspects and use of the following reactions in organic synthesis: Passerini-Ugi; Hantsch; Biginelli; Doebner-Miller; Ritter; Jacobson; Betti; Robinson-Schopf; Barbier; Baylis-Hilmann; Ivanov and Suzuki coupling reaction.

SUGGESTED BOOKS

1. Stereochemistry of carbon compounds, E. L. Eliel, S. H. Wilen and L. N. Mander, John Wiley & Sons, 1994.
2. Stereochemistry, Potapov, MIR, Moscow, 1984.
3. Stereochemistry, Nasipuri, D, New Age, 1999.
4. Advanced organic chemistry, J. March, 4th Edn. John Wiley, 2008.
5. Organic Chemistry, R. E. Ireland Prentice-Hall India, New Delhi, 1975.
6. Some modern methods of Organic Synthesis, W. Caruthers, Cambridge Uni. Press London, 2nd Edn. 1998.
7. Stereochemistry of organic compounds- Principle and applications, D. Nasipuri, 2nd Edn., New Age International Publishers, 2001.
8. Principles and applications of asymmetric synthesis, G D Lin, Y M Li and A S C Chan, Wiley Interscience, 2001.
9. A textbook of organic chemistry, V. K. Ahluwalia and M. Goyal, Narosa Publishing House, New Delhi, 2000.
10. Organic synthesis: Special techniques, V. K. Ahluwalia and R. Aggarwal, Narosa, New Delhi, 2003.
12. Green Chemistry, environment friendly alternatives, R. Sanghi and M M Srivastava, Narosa, New Delhi, 2003
12. Green Chemistry-an introduction text, Royal Society of Chemistry, UK, 2002.
13. Organic chemistry Vol. 2, 6th Edn., I. L. Finar, Longman, 1992.
14. Crownethers & cryptands, G. W. Gokel, Monograph, The Royal Society of Chemistry, 1991.
15. Macrocyclic Polyether Chemistry, G. W. Gokel, S. M. Korzeniowski, Vol 1 to 3, Wiley, NY, 1978, 1981, 1987.
16. Phase Transfer Catalysis in Organic Synthesis, W. B. Weber, G. W. Gokel, Springer, Berlin, 1977.
17. Phase Transfer Catalysis, E. V. Dehmlov, S. S. Dehmlov, 2nd Edn., Verlagchemie, Wienheim, 1983.
18. Polymers as aids in Organic synthesis, N. K. Mathur, C. K. Narang and R. E. Williams, Academic Press, NY, 1980.

C-105: PHOTOCHEMISTRY (SOFT CORE)

36 Hours

UNIT-I

12h

Photochemistry:

Importance of Photochemistry, Laws of Photochemistry: Grothus –Draper Law, Stark-Einsteins Law, Laws of light absorption, Quantum yield and numerical problems. Photochemistry and spectroscopy, units and dimensions. Electronic energy states of atoms, term symbols for atoms, energy levels for the electronic configuration of carbon and oxygen illustrating spin orbit coupling and Hunds rules, inverted multiplets as applied to simple atoms and also for inner transition metals, Laporte's selection rules. Physicochemical Properties of electronically excited molecules: Nature of changes on electronic excitation: acidity, dipole moment, redox potentials etc. Fates of excited species, Electronic, vibrational, rotational energies-potential energies diagram. Shapes of absorption band and Franck Condon principle.

UNIT-II

12h

Quantum mechanical formulation of Franck Condon, crossing of potential energy surfaces, Non crossing rule of Teller for potential energy surface. Emission spectra, fluorescence and phosphorescence

Environmental effect on absorption and emission spectra, solvent red shift and blue shift in absorption spectra. Experimental techniques to determine the intermediates in photochemical reactions

Classification of photochemical reactions, Rate constants and life times of reactive energy state Effect of light intensity on the rate of photochemical reaction Photo-fragmentation of photodissociation-Gas phase photolysis.

UNIT-III

12h

Photosensitized reaction, photofragmentation in liquid phase, photodegradation of polymers, Isomerization and other rearrangement reactions

Atmospheric photochemistry

Some current topics in photochemistry:

Semiconductors: Bonding and conductivity, mechanism of conductivity, energy bands in semiconductors, impurity semiconductors.

Photo voltaic effect: p-n junction solar cells, silicon cells, GaAs solar cells, schottky barrier solar cells.

Photoelectrochemistry: Introduction, efficiency of conversion of light to chemical and electrical energy, frequently measured quantities. Photosplitting of water using colloidal suspensions

Photocatalysis: Photocleavage of waste which are environmentally hazardous by using TiO_2, Photooxidation and photoreduction reactions

SUGGESTED BOOKS

1. Fundamentals of photochemistry, K.K. Rohatgi Mukhergee, Wiley Eastern Limited (1986)
2. Photochemistry, Carol E Wayne and Richard P Wayne, Oxford University Press (1996)
3. Introduction to Semiconductor Materials and devices M S Tyagi, John Wiley and sons (1991)
4. Organic Photochemistry, J. M. Cozen and B. Halton, Cambridge University Press (I st Edition) 1974
5. Molecular Reactions and Photochemistry, C H Deputy and D S Chapman, Prentice Hall India, New Delhi (1st Edition) , 1972.
6. Concepts of Inorganic photochemistry, A. W. Adamson and P D Fleischaves Wiley.
7. Elements of Inorganic Photochemistry G. J. Ferranti, Wiley.
8. Physical Chemistry, P. W. Atkins, Julio de Paulo ELBS 7th Edition (2002)

INORGANIC CHEMISTRY PRACTICALS

(4 days a week, 4 hours a day)

C-106 Inorganic Chemistry Practical-I

Semi micro qualitative analysis of mixtures containing two anions, two common cations and one less familiar elements: W, Mo, Ce, Th, Zr, V, U and Li.

C-107 Inorganic chemistry practical-II

Preparation and quantitative analysis of inorganic complexes:

1. Cis- and trans- potassium dioxalatodiaquachromium(III) complex [analysis of oxalate and chromium]
2. Hexamminecobalt(III)chloride [analysis of cobalt]
3. Mercurytetrathiocyanatocobaltate.
4. Preparation of pentamminechloro cobalt(III)chloride.

C-108 Inorganic Chemistry Practical-III

Gravimetric analysis

1. Gravimetric determination of Fe in iron ore as Fe_2O_3.
2. Gravimetric determination of Ni in Cu and Ni solution.
3. Gravimetric determination of Fe in Fe and Cr solution.
4. Total gravimetric estimation of Fe and Al.
5. Gravimetric estimation of Cu in Cu and Fe solution.
6. Gravimetric estimation of Cu in Cu and Zn solution.

C-109 Inorganic Chemistry Practical-IV

Volumetric analysis

1. Volumetric estimation of Ca and Mg in Dolomite solution.
2. Volumetric estimation of Cu in Cu and Ni (German Silver).
3. Volumetric estimation of Fe in Cu and Fe solution.
4. Volumetric estimation of Zn in Cu and Zn solution.
5. Volumetric estimation of Ni in Ni and Zn solution.

Suggested Books:

1. Vogel's Text book of Qualitative Chemical Analysis, J. Bassett, G. H. Jeffery and J. Mendham, ELBS (1986).
2. Vogel's text book of Quantitative Chemical Analysis, 5th Edition, J. Bassett, G. H. Jeffery and J. Mendham, and R. C. Denny, Longman Scientific and Technical (1999).
3. Inorganic Semimicro Qualitative Analysis, V. V. Ramanujam; The National Pub. Co. (1974).
4. Practical Inorganic Chemistry, G. Marr and B. W. Rockett, Von Nostrand Reinhold Co., London (1972).

ORGANIC CHEMISTRY PRACTICALS
(4 days a week, 4 hours a day)

C-106 Organic Chemistry Practical-I

Preparation (one stage)

1. Cannizarro reaction: Benzaldehyde.
2. Fries rearrangement: Phenyl acetate.
3. Friedel-Crafts reaction: Benzene and Acetyl chloride.
4. Sandmeyer reaction: 4-Chlorotoluene from 4-toluidine.
5. Pechmann reaction: Resorcinol and ethylacetoacetate.
6. Oxidation of Cyclohexanol.
7. Preparation of S- Benzylisothiuronium chloride.
8. Synthesis of *p*-iodonitrobenzene
9. Synthesis of N-Phenyl-2,4-dinitroaniline.
10. Synthesis of 2,4,6-tribromoaniline.
12. Synthesis of 2,4-dichlorophenoxyacetic acid.

C-107 Organic Chemistry Practical-II

Qualitative analysis

Systematic analysis and identification of organic compounds.

C-108 Organic Chemistry Practical – III

Preparation (Two and three stages)

1. 2,4-Dinitrophenylhydrazine from chloronitrobenzene.
2. Anthranilic acid from phthalic acid.
3. Benzanilide from benzophenone.
4. Benzilic acid from benzoin.
5. Synthesis of Acridone.
6. Synthesis of Hydantoin.

C-109 Organic Chemistry Practical-IV

Quantitative analysis

1. Titrimetric estimation of amino acids.
2. Saponification value of oil.
3. Estimation of glucose by Feighling's method.
4. Estimation of keto group.
5. Estimation of phenols.
6. Iodine value of oil (chloramine-T method).

SUGGESTED BOOKS

1. Laboratory manual of Organic Chemistry- B. B. Dey, M V Sitaraman and T R Govindachari, Allied Publishers, New Delhi, (1996).
2. Practical Organic Chemistry – Mann and Saunders, (1980).
3. Text Book of Practical Organic Chemistry- A. I. Vogel, (1996).

4. Test Book of Quantitative Organic Analysis- A. I. Vogel, (1996).
5. A Handbook of Organic Analysis – Clarke and Hayes, (1964).
6. Comprehensive practical organic chemistry : Preparation and quantitative Analysis, V. K. Ahluwalia, R. Aggarwal, Universities Press (India), 2000.
7. Comprehensive practical organic chemistry: Qualitative analysis, V. K. Ahluwalia, S. Dhingra, Universities Press (India), 2000.
8. An advanced course in practical chemistry, A. Ghoshal, B. Mahapatra and A. Kr. Nad, New central book agency, Calcutta, 2000.
9. Advanced practical organic chemistry, J. Mohan, Vol. I and II, Himalaya Publishing House, 1992.
10. Practical organic chemistry (Quantitative analysis), B. B. Dey, M. V. Sitaraman and T. R. Govindachari, Allied Publishers, New Delhi, 1992.

PHYSICAL CHEMISTRY PRACTICALS
(4 days a week, 4 hours a day)

C-106 Physical Chemistry Practical -I

1. Acid hydrolysis of methyl acetate at lab temperature.
2. Velocity constant for the saponification of ethyl acetate.
3. Verification of Beer's Law for Cu^{2+} ions
4. Verification of Beer's Law for Fe^{2+} ions
5. Estimation of Fe^{2+} ions concentration in the given solution by titration of FAS versus $KMnO_4$ through colorimetric method.
6. Estimation of Fe^{2+} ions concentration using EDTA through colorimetric method
7. Phase diagram of two component systems and determination of E_c , E_T and the determination of the composition of given unknown.
8. Determination of partial molar volume of solute –H_2O system by apparent molar volume method.
9. Determination of the viscosity of a mixture by apparent molar volume method.
10. Verification of Freundlich and Langmuir isotherm for adsorption of oxalic/acetic acid on activated charcoal.

C-107 Physical Chemistry Practical -II

Conductometric Experiments

1. Precipitation titration: conductometric titration of lithium sulphate versus $BaCl_2$
2. Conductometric titration of weak acid versus weak base.
3. Dissociation constant of weak acid (CH_3COOH) by conductometric method.
4. Determination of Equivalent conductance of a given strong electrolyte.
5. Conductometric titration of strong acid versus strong base.

Potentiometric Experiments

6. Determination of single electrode potential of Cu^{2+}/Cu and estimate the given unknown concentration.
7. Determination of single electrode potential of Zn^{2+}/Zn and estimate the given unknown concentration.
8. Titration of $AgNO_3$ versus KCl.
9. Titration of weak acid against a strong base using quinhydrone electrode and calculation of pKa and Ka values of the weak acid.
10. Determination of pH of a buffer by using quinhydrone electrode and comparison of the pH values obtained with glass electrode.

C-108 Physical Chemistry Practical -III

1. Study the hydrolysis of methyl acetate in presence of two different concentrations of HCl and report the relative strength.
2. Study the hydrolysis of methyl acetate in the presence of HCl at different temperatures and report the energy of activation.
3. Determination of dissociation constant of a given indicator by colorimetric method.
4. Study of kinetics of autocatalytic reaction between $KMnO_4$ versus oxalic acid.
5. Determination of degree of hydrolysis of aniline hydrochloride at room temperature and calculation of dissociation constant of the base by pH metry
6. Study of variation of viscosity of a liquid with temperature, determine the constant A and B.

7. Analysis of a binary mixture of two miscible liquids and to determine the composition of the given unknown mixture.
8. Determination of pH of acetic acid with sodium acetate buffer by pH metry method.
9. Determination of pH of formic acid with sodium formate buffer by pH metry method.
10. Evaluation of Arrehenius parameter for the reaction between $K_2S_2O_8$ versus KI (first order)

C-109 Physical Chemistry Practical -IV

Conductometry

1. Acid mixture versus NaOH
2. Weak acid with salt versus NaOH
3. Strong acid with salt versus NaOH
4. Determination of strength of HCl, CH_3COOH and $CuSO_4$ versus NaOH by pH metry
5. To determine the acidic and basic dissociation constant of an amino acid and determination of isoelectric point by pH metry.

Potentiometry

6. $K_2Cr_2O_7$ versus FAS
7. Acid mixture versus NaOH
8. $KMnO_4$ versus FAS
9. Determination of dissociation constant of H_3PO_4 using potentiometric method.
10. Determination of pKa value of phosphoric acid by pH meter.

SUGGETED BOOKS

1. Findlays practical physical chemisty revised by P. B. Levitt, Longman's London (1966).
2. Experiments in Physical Chemistry by Shoemaker and Garland, McGraw Hill International Edn. (1966)
3. Advanced Practical Physical Chemistry by J. B. Yadav, Goel Publications Meerut (1988)
4. Senior Practical Physical Chemistry by B. C. Kosla, Simla Printers New Delhi (1987)
5. Experimental Physical Chemistry by Daniel et al., McGraw Hill, New York (1962).
6. Practical Physical Chemistry by A.M James and P. E. Pritchard, Longman's Group Ltd (1968)
7. Experimental Physical Chemistry by Wilson, Newcombe & others, Pergamon Press, New York (1962)
8. Experimental Physical Chemistry by R. C. Behra and B Behra, Tata McGraw, New Delhi (1983)
9. Experimental Physical Chemistry by V. D. Atavale and Parul Mathur, New Age International, New York (2001)
10. Physical Chemistry Laboratory Principles and Experiments by H. W. Salberg J. I. Morrow, S. R. Cohen and M. E. Green Macmillan publishing Co .new York.
11. Practical's in physical chemistry A. Modern Approach by P.S Sindhu, Mac. Millan Publishers Delhi (2006).

SECOND SEMESTER

C-201: INORGANIC CHEMISTRY- II

52 hours

UNIT-I

Metal-Ligand equilibria in solution- Step-wise and overall formation constant and their relationship, trends in step-wise constant, kinetic and thermodynamic stability of metal complexes, factors affecting the stability of metal complexes with reference to the nature of the metal ion and ligand, chelate effect, macrocyclic effect and their thermodynamic origin. Determination of binary formation constant by pH metry, spectrophotometry, polarography and ion exchange methods.

Structure and bonding- Structure and bonding in hydride, dihydrogen, dioxygen, isocyanide, CO, NO, N_2 and tertiary phosphine complexes of transition metals. **13h**

UNIT-II

Metal- ligand bonding- Stereoisomerism- coordination numbers 3 to 8. Crystal field theory, salient features, spectrochemical series, splitting of d-orbitals in tetragonal, square planar, trigonal bipyramidal and square-pyramidal geometry, applications of CFT- colours of transition metal complexes, magnetic properties of octahedral complex, distortion of octahedral complex, CFSE and their uses, factors affecting CFSE, limitations of CFT, experimental evidence for metal-ligand covalent bonding in complexes, nephelauxetic effect, Ligand Field Theory, MO theory: tetrahedral and octahedral complexes (including π-bonding), angular overlap model.

Stereochemical non-rigidity, self assembly in supramolecular chemistry. **13h**

UNIT-III

Electronic spectra of coordination compounds- Spectroscopic ground states, selection rules, term symbols for d^n ions, Racah parameters, Orgel, Correlation and Tanaube-Sugano diagrams, spectra of 3d metal-aqua complexes of trivalent V, Cr, divalent Mn, Co and Ni, $CoCl_4^{2-}$, calculation of Dq, B and β parameters, CT spectra.

Spectral properties of Lanthanide and Actinide metal complexes. **13h**

UNIT-IV

Magnetic properties of coordination compounds- Types of magnetic behaviour, magnetic susceptibility and its determination- Gouy, Faraday, VSM method. Diamagnetic correction, orbital contribution, spin-orbital coupling, ferro- and antiferromagnetic coupling, spin-crossover. Magnetic properties of Lanthanide and Actinide metal complexes.

Photochemical reactions of transition metals complexes: Basic photochemical processes, Kasha's rule, quantum yield, Jabolnskii diagrams, photo substitution reactions, photo-redox reactions, ligand photoreactions, photoreactions and solar energy conversion.

13h

SUGGESTED BOOKS

1. Basic Inorganic Chemistry- F. A. Cotton, G. Wilkinson and P. L. Gaus; John Wiley and sons. Inc, 6th edition (1999).
2. Chemistry of elements- N. N. Greenwood and A. E. Earnshaw, Butterworth Heinemann (1997).
3. Inorganic Chemistry IV edition; J. E. Huheey, E. A. Keiter and R. L. Keiter, Addison; Wesley (1993).
4. Inorganic Chemistry, II edition, D. F. Shriver, P. W. Atkins and C. H. Langford, ELBS; Oxford University Press, 1994.
5. Inorganic Electronic spectroscopy, A. B. P. Lever, Elsevier. (1968).
6. Magnetochemistry, R.L. Carlin, Springer Verlag.
7. Electronic Absorption Spectroscopy and related Techniques, D. N. Sathyanarayana, University Press (2001).
8. Inorganic Chemistry A Unified Approach by W. W. Porterfield, Elsevier 2005 2nd edition.
9. Textbook of inorganic chemistry by G. S. Sodhi, Viva books Pvt. Ltd (2011).

C-202: ORGANIC CHEMISTRY- II

52 Hours

UNIT-I

Aromatic Substitution Reactions **12h**

Electrophilic Substitution Reactions: The arenium ion mechanism. Orientation and reactivity. Energy profile diagrams. The *ortho*/*para* ratio, *ipso* attack, orientation in other ring systems.Quantitative treatment of reactivity in substrates and electrophiles.Effect of leaving group.Amination, sulfonylation reactions; Diazonium coupling, Vilsmeier-Haack reaction, Gatterman reaction, Gatterman-Koch reaction and Hoesch reaction.

Nucleophilic substitution reactions: The SNAr, SN1, benzyne and SRN1 mechanisms. Reactivity: effect of substrate structure, leaving group and attacking nucleophile. Goldberg reaction, Bucherer reaction, Schiemann reaction, von Richter reaction, Sommelet-Hauser and Smiles rearrangements.

UNIT-II

Addition Reactions **12h**

Addition to carbon-carbon multiple bonds: mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals. Regio, stereo- and chemoselectivities.Orientation and reactivity. Addition to cyclopropane ring.Hydrogenation of double and triple bonds, hydrogenation of aromatic rings.Addition of alkenes and/or alkynes to alkenes and/or alkynes. Ene synthesis. Michael reaction.

Addition to carbon-heteroatom multiple bonds: Mechanism of metal hydride reduction (NaH, LiH, $LiAlH_4$, $NaBH_4$) of saturated and unsaturated carbonyl compounds, acids, esters and nitriles. Addition of Grignard reagents and organolithium reagents to carbonyl compounds and unsaturated carbonyl compounds. Conversion of aldehydes to nitriles. Hydrolysis of nitriles and addition of amines to isocyanates. Formation of xanthates. Wittig, Mannich and Stobbe reactions.

UNIT-III

Elimination Reactions **4h**

The E2, E1 and E1cB mechanisms and their spectrum.E2C and E2H mechanisms.Orientation of the double bond.Reactivity-effects of substrate structure, attacking base, the leaving group and the medium.Mechanism and orientation in pyrolytic elimination reactions (including Chugaev reaction).

Rearrangements **12h**

Wagner-Meerwein, Pinacol-Pinacolone, Fries, Wolff, Beckmann, Hofmann, Curtius, Lossen and Schmidt rearrangements. Benzil-benzilic acid rearrangement, Arndt-Eistert reaction, Tiffeneau-Demjanov reaction, Firtsch-Buttenberg-Wiechell rearrangement. Stevens, Wittig and Favorskii rearrangements, Dienone-phenol, Baker-Venkatraman rearrangement. Baeyer-Villiger oxidation. Neber rearrangement. Benzidine rearrangement,

UNIT-IV

Amino acids and Peptides **12h**

Synthesis and reactions of amino acids.

Classification and nomenclature of peptides.Sanger and Edman methods of sequencing.Cleavage of peptide bond by chemical and enzymatic methods.
Peptide synthesis- Protection of amino group (Boc-, Z- and Fmoc-) and carboxyl group as alkyl and aryl esters. Use of DCC, EEDQ, HOBt and active esters, acid halides, anhydrides in peptide bond formation reactions. Deprotection and racemization in peptide synthesis.Solution and solid phase techniques. Synthesis of oxytocin, gramicidin, enkephalins, LH-RH.
Introduction to peptidomimetics.

SUGGESTED BOOKS

1. Advanced Organic Chemistry – Reactions, Mechanism and Structure, Jerry March, John Wiley (2008).
2. Advanced Organic Chemistry, F. A. Carey and R. J. Sundberg, Plenum (1990).
3. A Guide Book to Mechanism of Organic Chemistry, Peter Sykes, Longman (2000).
4. Structure and Mechanism of Organic Chemistry, C. K. Ingold, Cornell University Press.
5. Organic Chemistry, R. T. Morrison and R. N. Boyd, Prentice-Hall (1998).
6. Modern Organic Reactions, H. O. House, Benjamin (1972).
7. Principles of Organic Synthesis, ROC Norman and J. M. Coxon, Blackie Academic and Professional (1996).
8. Stereochemistry of Organic Compounds, D. Nasipuri, New-Age International (1999).
9. Stereochemistry of Carbon Compounds, E. L. Eliel, S. H. Wilen and L. N. Mander, John Wiley (1994).
10. Organic Chemistry, Volumes I and II, I L Finar, Longman. (1999).
11. Medicinal Chemistry, A Kar, Wiley (2000).
12. Peptides Chemistry: A practical text book, M. Bodansky, Springer-Verlag NY, 1988.
13. Solid-phase peptide synthesis: A practical approach-E. Artherton & R.C. Sheppard, I R L, Oxford Univ. Press, 1989.
14. Peptides: Chemistry and Biology, N Selwad and H.-D. Jakubke, Wiley-VCH, 2002.

C-203: PHYSICAL CHEMISTRY- II

52 Hours

UNIT-I

Thermodynamics-I **13h**

Thermodynamics: Concepts of partial molar properties – partial molar free energy, chemical potential, partial molar volume and its significance. Gibbs-Duhem equation , Gibbs-Duhem-Margulus equation. Determination of partial molar volume : Graphical method, intercept method and Apparent molar volume method. Concept of fugacity; Determination of fugacity by graphical method and compressibility factor method. Activity and activity coefficient : Determination of activity coefficient by EMF and solubility method. Thermodynamics of non-ideal system-Excess thermodynamic function, G^E ,S^E , H^E etc.

Phase Rule : Derivation of phase rule from the concept of chemical potential. Application of Phase Rule to three components system :Principle of triangular diagram : Plots for a mixture of three liquids consisting of one ,two and three pairs of partially miscible liquids.

Statistical Thermodynamics: Objectives of statistical thermodynamics, Concept of distributions, Types of ensembles. Thermodynamic probability, Most probable distribution Law – Partition Function, (Definition and significance): Molar and molecular partitions-translational, rotational , vibrational and electronic partition functions- Relation between thermodynamic functions (E, H,S,G and C_v) and the partition functions.

UNIT-II

Thermodynamics-II **13h**

Sackur-Tetrode equation for entropy of translation function. Relation between equilibrium constant and partition function.

Different Distribution Laws:Types of Statistics : Maxwell – Boltzmann , Bose-Einstein and Fermi-Dirac statistics. Derivation of the equations for above three distribution Laws. Comparision of Bose-Einstein and Fermi-Dirac statistics with Maxwell – Boltzmann statistics. Problems and their Solutions.

Non-equillbrium Thermodynamics :

Thermodynamic criteria for non-equillibrium states-Phenomenological Laws and Onsager's reciprocity relations, Coupled and Non-coupled reactions, Entropy production and entropy flow. Electro kinetic Phenomenon.

Postulates and methodologies: Uncompensated heat and thermodynamics fuction production. de-Donder's inequality. Rate of entropy production. Transformations of the generalized fluxes and forces : eg., Chemical reaction, heat flow, Diffusion or material flow, flow of electric current.

UNIT-III

13h

Electrochemistry-I

Elcetrochemistry of solutions: Ionic atmosphere, Debye-Huckel theory for the problem of activity coefficient, Debye-Huckel limiting Law, Debye-Huckel equation for appreciable concentration, Debye-Huckel Onsagar conductance equation and its extension to ion solvent interations, Debye-Huckel Bjerrum mode, Ion association, triple ions, triple ions and conductance minima. Thermodynamics of electrified interface, derivation of electro capillary Lipmann's equation, surface excess, thermodynamic aspects of surface excess. The method of

determination and measurement of interfacial tension as a function of applied potential difference across the interface.

UNIT-IV

Electrochemistry-II **13h**

Structure of electrified interface: Helmholyz theory, Guoy- Chapman theory, Stern model.

Overpotential: Concentration overpotential and activation overpotential, Derivation of Butler-volmer equation.

Electrocatalysis: Definition and Influence of various parameters.

Quantum aspects of charge transfer at electrode solution interface, quantization of charge transfer, tunneling of electrons for hydrogen evolution with reference to electrocatalysis.

Polarography: Ilkovic equation, half wave potential and its significance, qualitative and quantitative estimation of metal ions.

Semiconductor- solution interface: Theory of double layers at semiconductor- electrolyte interface.

SUGGESTED BOOKS

1. Molecular thermodynamics, Donald A. Mc Quarrie, John D. Simon University Science Books California, (1999).
2. Thermodynamics for Chemists, by S. Glasstone, East-West Press, New Delhi, (1960).
3. Thermodynamics,by Rajaraman and Kuriacose, East-West Press, (1986).
4. Statistical Thermodynamics, M. C. Gupta (Wiley Eastern Ltd.) 1993.
5. Elementary Statistical Thermodynamics, N. D. Smith, Plenum Press, NY, (1982).
6. Elements of Classical and Statistical Thermodynamics, L. K. Nash, Addison-Wiley (1979).
7. Thermodynamics, Statistical Thermodynamics and Kinetics by Thomas Engel & Philip Reid, Pearson Education inc. (2007)
8. Modern Electrochemistry Vol-1 and 2 J. O. M Bockris and A. K. N. Raddy, Plenum NewYork (1978)
9. An introduction to electrochemistry- Samuel Glastone East-West edition New Delhi (1942)
10. Text book of physical chemistry Samuel Glastone , 2nd edition, Mac Millan India Ltd (1991)
11. Electrochemistry, Principles and applications, Edmund, C. Potter, Cleaver-Hume press London (1961).
12 Principles and applications of Electrochemistry- D. R. Crow 3rd edition Chapmanhall London (1988)

C-204: SPECTROSCOPY-I

52 Hours

UNIT-I

Symmetry and Group Theory in Chemistry **12h**

Definition of groups, subgroups, cyclic groups, conjugate relationships, classes, simple theorems in group theory. Symmetry elements and symmetry operations, point groups, Schöenflies notations, representations of groups by matrices, reducible and irreducible representations, characters of representations, Great Orthogonality Theorem (without proof) and its applications, character tables and their uses (representations for the C_n, C_{nv}, C_{nh}, D_{nh} etc groups to be worked out explicitly) Mulliken symbols for irreducible representations

Direct products, Applications of group theory to quantum mechanics- identifying non-zero matrix elements, derivation of the orthonormalization conditions

Unifying principles **3h**

Interaction of electromagnetic radiation with matter- time-dependent perturbation theory, transition moment integral, selection rules- symmetry and spin forbidden transitions

UNIT-II

Microwave Spectroscopy **6h**

Rotations of molecules, rigid diatomic molecule- rotational energy expression, energy level diagram, rotational wave functions and their symmetry, selection rules, expression for the energies of spectral lines, computation of intensities, effect of isotopic substitution, centrifugal distortion and the spectrum of a non-rigid rotor.

Rotational spectra of polyatomic molecules- linear, symmetric top and asymmetric top molecules

Stark effect, techniques and instrumentation

Infrared Spectroscopy-I **6h**

Vibrations of molecules, harmonic and anharmonic oscillators- vibrational energy expression, energy level diagram, vibrational wave functions and their symmetry, selection rules, expression for the energies of spectral lines, computation of intensities, hot bands, effect of isotopic substitution

Diatomic vibrating rotor, Born-Oppenheimer approximation, vibrational-rotational spectra of diatomic molecules, P, Q and R branches, breakdown of the Born-Oppenheimer approximation.

UNIT-III

Infrared Spectroscopy-II **6h**

Vibrations of polyatomic molecules: Normal coordinates, translations, vibrations and rotations, vibrational energy levels and wave functions, fundamentals, overtones and combinations

Vibration-rotation spectra of polyatomic molecules- parallel and perpendicular vibrations of linear and symmetric top molecules

Techniques and instrumentation, FTIR

Raman Spectroscopy **7h**

Classical theory of the Raman effect, polarizability as a tensor, polarizability ellipsoids, quantum theory of the Raman effect, Pure rotational Raman spectra of linear and aymmetric top molecules, vibrational Raman spectra, Raman activity of vibrations, rule of mutual exclusion, rotational fine structure- O and S branches, Polarization of Raman scattered photons

Structure determination from Raman and IR spectroscopy-AB_2 and AB_3 molecules

Techniques and instrumentation

UNIT-IV

Electronic Spectroscopy **12h**

Born-Oppenheimer approximation, vibrational coarse structure, intensities by Franck-Condon principle, Dissociation energy, rotational fine structure, Fortrat diagram, pre-dissociation

Electronic structure of diatomic molecules- basic results of MO theory, classification of states by electronic angular momentum-σ,π,δ, and ϕ molecular orbitals, selection rules, spectrum of singlet and triplet molecular hydrogen

Electronic spectra of polyatomic molecules- localized MOs, spectrum of HCHO, change of shape on excitation

Decay of excited states- radiative (fluorescence and phosphorescence) and non-radiative decay, internal conversion

SUGGESTED BOOKS

1. Chemical Applications of Group Theory, F. A. Cotton, Wiley Eastern (1976).
2. Molecular Symmetry, D. S. Schonland, Van Nostrand (1965).
3. Introduction to Molecular Spectroscopy, C. N. Banwell, TMH Edition (1994).
4. Introduction to Molecular Spectroscopy, G. M. Barrow, McGraw Hill (Int. Students Edition) (1988).
5. Molecular Spectroscopy, J. D. Graybeal, McGraw Hill (Int. Students Edition) (1990).
6. Spectroscopy, Vols. 1-3, B. P. Straughan and W. Walker, Chapman Hall (1976).

C-205: SOFT CORE: MATHEMATICS FOR CHEMISTS

36 Hours

UNIT-I

12h

Vectors: vectors, dot and cross products; scalar and vector triple products and their applications. Tensors and their applications.

Matrix Algebra: Review of different types of matrices (including Hermetian and skew Hermetian); matrix addition and multiplication; determinant of a square matrix, transpose, adjoint and inverse of a square matrix. Solution to system of linear equation (a) by matrix method and (b) by Cramer's Rule. Characteristic equation of a square matrix, eigenvalues and eigenvectors.

UNIT-II

12h

Calculus: Rule for differentiation; Chain rule (for $f(x)=U^n$, sin u, log u etc). Implicit differentiation and parametric differentiation and successive differentiation of order 2 (for explicit functions only).

Applications of differentiation:

Derivative as a slope of the tangent, derivative as a rate measure-velocity and acceleration. Increasing and decreasing functions-Maxima and minima-second derivative test-point of inflections-problems restricted to polynomial.

UNIT-III

12h

Integrations: Basic rules-simple substitution-Method of partial fractions-Integration by parts. Define integral and application to areas of plane curves.

Functions of several variables: partial derivatives; co-ordinate transformation from cartesian co-ordinates to spherical and cylindrical coordinates and vice-versa.

Elementary differential equation: Variable separable, exact first order equations, linear and homogeneous equation.

Second order homogeneous differential equation with constant coefficients f(D), y=0. Solution of differential equation by power series method.

Fourier series: Simple problems.

Probability: Review of permutations and combinations. Probability and addition theorem for mutually exclusive events and multiplication theorem for independent events.

Curve fitting-Method of least squares.

SUGGESTED BOOKS

1. Mathematical Preparation for physical chemistry, F. Daniells, M.Graw Hill Inc., US, 1959.
2. Mathematics for chemists, D. M. Hirst, Chemical Publishing Company Incorporated, New York, 1979.
3. Mathematics for chemists, P. G. Francis, Springer, 2011.
4. Basic Mathematics for chemists, P. Tebutt, Wiley-Blackwell, 1994.
5. Calculus and analytic geometry, 9th edition, G. B. Thomas, R.L. Finney, Addison-Wesley Publishing Company, Inc. 1996.
6. Short Course in differential equations, Rainvilles and Bedient, IBH publishers, 1968.
7. Mathematics for chemistry, G. Doggett and B. T. Sutcliffe Longmann Publishers, 1995.

C 206, C 207, C 208 and C209
Practicals

(4 hrs per day, 4 days per week)

Inorganic Chemistry Practicals - I, II, III & IV
Organic Chemistry Practicals - I, II, III & IV
Physical Chemistry Practicals - I, II, III & IV

Experiments are as in first semester. Every student will carry out experiments in each of the three branches of chemistry on a rotation basis from 1st to 3rd Semester.

THIRD SEMESTER
ANALYTICAL CHEMSITRY SPECIALISATION

C - 301 AC PRINCIPLES OF CHEMICAL ANALYSIS

52 Hours

UNIT-I

Acid – Base Titrations: **5h**

Basic principles, Titration curves for mono functional acids and bases, pH calculations, theory of indicators, fractions of phosphoric acid species as a function of pH. Titration curves for polyfunctional acids [H_3PO_4], polyamines and amino acid systems.

Redox Titrations: **6h**

Nernst equation, Standard & formal potentials. Titration curves, end point signals, Indicators, criteria for the selection of indicators. Feasibility of redox titration. Titration of multicomponent system. Adjustment of analyte's oxidation state. Applications: Oxidants such as Permanganate, dichromate, Ce (IV), bromate, Iodates.

UNIT-II

Precipitation titrations: **5h**

Solubility product. Theoretical principles: Titration curves, end point signals, Mohr, Volhard and adsorption indicators. Applications: Estimation of F^-, K^+, CO_3^{2-}, $C_2O_4^{2-}$, acetylenes and mixture of halides

Complexometric titrations: **6h**

Complexometric titrations with particular reference to EDTA titrations, suitability of polydentate ligands as titrants, expressions for the different forms of EDTA in solution as a function of pH, conditional stability constants, derivation of titration curve, effect of pH and second complexing agent on the conditional stability constant and titration curve. Selectivity by pH control, masking and demasking, metal ion indicators, types of EDTA titrations, titrations involving monodentate

UNIT-III

Karl-Fischer titrations: **5h**

Stoichiometry of the reaction, preparation of the reagent, titration method, standardization of the reagent using water-in-methanol, determination of water in samples, interference and their elimination, application to quantitative analysis of some organic compounds- alcohols, carboxylic acids, acid anhydrides and carbonyl compounds.

Non-Aqueous titrations: **5h**

Acid –base titrations in non-aqueous solvents- classification of solvents, leveling and differentiating solvents, acidic and basic titrants, methods of titration. Titrations in glacial acetic acid and ethylene diamine, applications of non-aqueous titrations.

Gravimetric analysis: **5h**

Formation and treatment of precipitates, co-precipitation, homogeneous precipitation, important precipitating agents and their significance in inorganic analysis.

UNIT-IV

Kinetic methods of analysis: 5h

Rate laws, psuedo first order kinetics, types of kinetic methods, fixed time methods. Applications of catalytic and non-catalytic kinetic methods.

Electroanalytical techniques 10h

Membrane indicator electrodes- Classification of membranes, properties of ion-selective membranes, the glass electrode for P^H measurements, glass electrodes for other cations, crystalline membrane electrodes,liquid membrane electrodes. Ion-selective field-defect transistors (ISFETs): Mechanisam of ISFET ion-selective behavior, application of ISFETs. Molecular selective electrode systems: Gas-sensing probes, biocatalytic membrane electrodes, disposable multiplayer p-ion systems.

SUGGESTED BOOKS

1. Fundamentals Of Analytical Chemistry-Skoog, West And Holler 7th Edition Saunders College Publishing Int.Ltd. (1996)
2. Modern methods of Chemical analysis-Pecsok, Shields, Cairns and McWilliams (2nd edition), John Wiley and Sons (1976).
3. Vogel's Textbook of Quantitative Inorganic Analysis, Bassett, Denney, Jeffery and Mendham, (4th edition) ELBS (1989).
4. Analytical Chemistry-G.D.Christian (5th edition) John Wiley & sons (1946).
5. Treatise on analytical Chemistry-Kolthoff, Elving and Krivan (2nd edition) John Wiley & Sons (1986).
6. Commercial methods of analysis-Snell and Biffen, McGraw Hill, (1944)
7. Hand Book Of Instrumental Techniques For Analytical Chemistry, Frank Settle, Prentice Hall PTR (1997)
8. Fundamentals of Analytical Chemistry, Eigth Edition, Skooj, West, Holler and Crouch; Thomson Asia Pvt. Ltd (2004).

C - 302 ADVANCED ANALYTICAL TECHNIQUES

(Common to Inorganic and Analytical Chemistry)

52 Hours

UNIT-I

14h

Absorption Spectroscopy: absorption, emission, fluorescence phenomenon, principles and differences, Flame AAS, Instrumentation, different types of nebulizers, Nonflame techniques, GAAS, electrothermal vapourisers, graphite furnace, cold vapour AAS, radiation sources, HCL, EDL, TGL etc. detectors, photoemmissive cells, PMT, photodiodes, Interferences, spectral, chemical, matrix, background absorption, correction methods, deuterium arc, zeeman effect, Smith-Hieftje methos, single beam and double beam instruments, evaluation procedures, applications of AAS,

UNIT-II

12h

Atomic Emission Spectroscopy: Emission-priciple, Inductively coupled plasma optical emission spectrometry, theory, ICP characteristics, sample introduction methods, tourch configuration and view modes, analytical performance.merits and limitations of AES over AAS, Detection limit, application to elemental analysis, Microwave induced plasma systems in atomic spectrometry, principal processes, applications. Mass spectrometry in the analysis of inorganic compounds-different techniques, applications

UNIT-III

12h

Electroanalytical Techniques: Electrode Potential, Currents in Electrochemical cells, Potentiometric titrations. Electrogravimetry-faraday's laws of electrolysis, Coulometry, Coulometric titrations. Voltammetry- principle, DME-advantages,limitations, HydrodynamicVoltammetry, Cyclic voltammetry-priciple, conditions for reversible, quasi reversible and irreversible reactions Anodic stripping voltammetry-priciple and applications, Polarography, Pulse polarography, Amperometry-titrations, different titration curves,applications, numerical problems on all these techniques .

UNIT-IV

14h

Thermal Methods of Analysis: Principle, methodology and applications: thermogravimetric and differential thermal analysis, differential scanning calorimetry; Thermo-mechanical and dynamic mechanical analysis ; thermometric titrations. Thermal stability of polymers, applications, decomposition patterns, decomposition reactions-examples.

Biomolecules-Analysis: Introduction, single biomolecule detection and characterization, Fluorescence, principle, factors influencing fluorescence, fluorescence based biosensors, fluoroimmunosensors, Mass spectrometry-principle, sample preparation, probe tip, MALDIMASS, types of ion separation, instrumentation-types, applications in structural biology, Application of NMR spectroscopy in the analysis of biomolecules, Raman spectroscopy- phenomenon, merits and limitations, application to biomolecules,

Voltammetry in Vivo for chemical analysis of neurotransmitters in central nervous system

SUGGESTED BOOKS

1. Analytical Chemistry. Gary D Christian, 5th Edition, John – Wiley and Sons Inc., (1994)
2. Fundamentals of Analytical Chemistry.D. A. Skoog, D. M. West and F. J. Holler, 7th Edition, Saunders College Publishing (1996).
3. Instrumental methods of Analysis.H. H. Willard, L. L. Merrit , J. A. Dean and F. A. Set, CBS Publishers (1996).
4. Instrumental methods of Chemical Analysis, G. W. Ewing, 5th edition, McGraw-Hill, New York, 1988.
5. Electrochemical methods: A.J. Bard & l. R. Faulkner, 2nd edition, Wiley, New York, 2000.
6. Vogel's text book of Quantitative Chemical analysis 5th edition, Ed., Jeffery et. al ELBS/Longman, 1989
7. Encyclopedia of Analytical Chemistry: Ed. By R.A. Meyers Vol. 1 – 15, John Wiley, 2000.
8. Fundamentals of Instrumental Analysis, Skoog, D. M. West and F. J. Holler, 8th Edition, Saunders College Publishing (2004).

C-303 SPECTROSCOPY-II

(Common to Analytical, Inorganic and Physical Chemistry Students)

52Hours

UNIT-I

13h

Ultraviolet and Visible Spectroscopy

Classification of electronic transitions, Terminology, Substituent and solvent effects, UV spectral study of alkenes, polyenes, enones and aromatic compounds. Emprical rules for calculating lamda max.

Vibrational Spectroscopy

Sampling techniques, Group frequencies, factors affecting group frequencies, Bond order, Mass effect, Conjugation, Inductive, resonance, steric effects, intramolecular interactions. Application of IR in the study of H-bonding and tautomerism. Complimentarity of IR and Raman. Identification of the following organic compounds by IR: Alkanes, Alkenes, Alkynes, Aromatic compounds, Aldhydes, Ketones, Alcohols, Acids and its derivatives; Amines, Esters, Alkyl halides and Nitro compounds; Problems using UV and IR.

UNIT-II

13h

Nuclear Magnetic Resonance Spectroscopy

Introduction, Magnetic properties of nuclei-Resonance condition, Nuclear spin, population of nuclear spin levels and NMR isotopes, Relaxation methods, Instrumentation and sampling handling; Classical approach and FT-NMR.

Chemical shift, Factors influencing chemical shifts : electronegativity and electrostatic effects; Mechanism of shielding and deshielding in alkanes, alkyl halides, alkenes, aromatic compounds, carbonyl compounds and annulenes. Pascals triangle-low and high resolution, Reference compounds (internal and external reference compounds) Karplus Curve, Diamagnetic and Paramagnetic effects and Magnetic anisotropy. Equivalence of protons-chemical and magnetic equivalence; Spin systems: First order and second order coupling of AB systems, Simplification of complex spectra. Problems.

Spin-spin interactions: Homonuclear coupling interactions - AX, AX_2, AX_3, AMX, AB types. Vicinal, germinal and long range coupling-spin decoupling; Chemical shift reagents and deuterium exchange; Stereochemistry and hindered rotations. Temperature effects.

CIDNP, Nuclear Overhauser effect (NOE), Factors influencing coupling constants and Relative intensities.

UNIT-III

13h

^{13}C NMR Spectroscopy

Types of CMR spectra-undecoupled, proton decoupled, Off-resonance decoupled (SFORD); Selectively decoupled and gated decoupled spectra. ^{13}C chemical shifts of alkanes, alkyl halides, alkenes, alkynes, alcohols, ethers, carbonyl compounds and aromatic compounds; Factors affecting the chemical shifts. Applications of **13** C NMR spectroscopy in confirmation of structure and stereochemistry of organic molecules and in determining the reaction mechanism and dynamic processes of organic reactions – examples.

Mass Spectrometry-I

Basic principles - instrumentation ;Ion production : Soft ionization methods: Low energy electron ejection; Chemical ionization; Ionization of large molecules : Fast-atom bombardment (FAB), Plasma desorption (PD) and Matrix Assisted Laser Desorption/ionization (MALDI); Electrospray ionization (ESI); Pyrolysis; Exact mass measurements (high resolution spectra); Tandem mass spectrometry (MS/MS); Combined techniques;

UNIT-IV

Mass Spectrometry-II **13h**

Classification of mass spectrometers: Magnetic field deflection: magnetic field only (unit resolution) and double focusing (electrostatic field and magnetic field); High resolution; Quadrapole mass spectrometers: i. quadrupole mass filter and quadrupole ion storage (ion trap) Time of flight mass spectrometers; FT-ICR (ion cyclotron resonance spectrometers); MS/MS (tandem mass spectrometry).

Mass spectrum: Unit mass molecular ion and isotope peaks; High resolution molecular ion; recognition of the molecular ion peak; Use of molecular formula;

Fragmentation of alkanes, alkenes, alkyl halides, alcohols, aldehydes, ketones (cyclic and acyclic compounds), acids, esters, ethers, amines, nitro and halo compounds, peptides; Nitrogen rule; Factors affecting cleavage patters; McLafferty rearrangement;

Composite problems; Use of HRMS to determine exact molecular weight of compounds;

Application of UV, IR, NMR and mass methods in the structural elucidation of organic compounds

SUGGESTED BOOKS

1. Application of absorption spectroscopy to organic compounds, J. R. Dyer, Prentice-Hall, New Delhi, 1969.
2. Organic spectroscopy, P. Laszlo and P. Strang, Harper and Row, New York, 1971.
3. Organic spectroscopy, W. Kemp, ELBS London, 2000.
4. Spectrometric identification of organic compounds, sixth edition, R. M. Silverstien, and F. X. Webster, 2004.
5. Introduction to spectroscopy, 3rd Edition, D. L. Pavia, G. M. Laupman and G. S. Kriz, Harcourt college publishers, 2001.
6. Interpretation of mass spectra, Fourth edition, F.W. McLafferty, F. Turecek, California, 1993.
7. Practical organic mass spectroscopy, 2nd edition, J R Chapman, John Wiley, NY, 1993,
8. The IR spectra of complex molecules, Vols.1 and 2, L J Bellamy, Chapman and halli, London, 1975.
9. Spectroscopic techniquies for organic chemists, J W Cooper, John Wiley, NY, 1980.
10. Bimolecular NMR Spectroscopy, J N S Evans, Oxford univ. 1995.
11. Mass spectroscopy a foundation course. K Downard, RSC, Cambridge, 2004.
12. Instruemental methods of analysis, H. H. Willard, L. L. Merrit, J. A. Dean and F.A. Settle, CBS Publishers and Distributors, 1986.

C304- OPEN ELECTIVE – NON-CHEMISTRY PAPER

ANALYTICAL CHEMISTRY PRACTICALS

C- 305 Analytical Chemistry Practical I (Organic Chemistry)
Preparations

1. Cannizarro reaction: Benzaldehyde.
2. Friedel-Crafts reaction: Benzene and Acetyl chloride.
3. Claisen-Schmidt reaction: Acetophenone and Benzaldehyde / acetone and benzaldehyde.
4. Sandmeyer reaction: p-Chlorotoluene from p-toluidine..
5. Preparation of S- benzylisothiuronium chloride.
6. Anthranilic acid from phthalic acid.
7. 2,4-Dinitrophenylhydrazine from chloronitrobenzene.
8. *m*-Nitrobenzoic acid from methyl benzoate.

C- 306 Analytical Chemistry Practical II (Organic Chemistry)
Quantitative analysis

1. Saponification value of oil.
2. Estimation of glucose.
3. Estimation of Keto group
4. Estimation of amines/phenols by acylation method.
5. Iodine value of oil.

SUGGESTED BOOKS

1. Laboratory manual of Organic Chemistry- B. B. Dey, M V Sitaraman and T R Govindachari, Allied Publishers, New Delhi, (1996).
2. Practical Organic Chemistry – Mann and Saunders, (1980).
3. Text Book of Practical Organic Chemistry- A. I. Vogel, (1996).
4. Test Book of Quantitative Organic Analysis- A. I. Vogel, (1996).
5. A Handbook of Organic Analysis – Clarke and Hayes, (1964).
6. Comprehensive practical organic chemistry : Preparation and quantitative Analysis, V.K. Ahluwalia, R. Aggarwal, Universities Press (India), 2000.
7. Comprehensive practical organic chemistry: Qualitative analysis, V.K. Ahluwalia, S. Dhingra, Universities Press (India), 2000.
8. An advanced course in practical chemistry, A. Ghoshal, B. Mahapatra and A.Kr. Nad, New central book agency, Calcutta, 2000.
9. Advanced practical organic chemistry, J. Mohan, Vol. I and II, Himalaya Publishing House, 1992.
10. Practical organic chemistry (Quantitative analysis), B. B. Dey, M V Sitaraman and T R Govindachari, Allied Publishers, New Delhi, 1992.
11. Laboratory Techniques in Organic Chemistry, V K Ahluwalia, Pooja Bhagat and Renu Aggarwal, I K international Publishing House, New Delhi, 2005.
12. Intermediates for Organic Synthesis, V K Ahluwalia, Pooja Bhagat, Ramesh Chandra and Renu Aggarwal, I K International Publishing House, New Delhi, 2005.

C- 307 Analytical Chemistry Practical –III

Chemical Analysis of ore samples:

Dissolution and Laboratory analysis of the following ore samples:

1) Analysis of haematite: Estimation of silica by gravimetry and iron by volumetry.

2) Analysis of Portland cement: Estimation of insoluble residue by gravimetry and CaO by volumetry
3) Analysis of bauxite :Estimation of silica by gravimetry and aluminium by gravimetry
4) Analysis of dolomite: Estimation of CaO and MgO by volumetry
5) Analysis of pyrolusite: Estimation of metallic hydroxides by gravimetry and manganese by volumetric estimation.

C- 308 Analytical Chemistry Practical – IV

Chemical Analysis of Alloy samples: Dissolution, sample preparation & Analysis.

1) Analysis of brass: Estimation of copper by gravimetry and zinc by EDTA titration
2) Analysis of bronze: Estimation of copper by volumetry and tin by gravimetry
3) Analysis of type metal: Analysis of lead by volumetry and tin by gravimetry
4) Analysis of chrome steel: Estimation of iron by volumetry and Cr by colorimetry
5) Analysis of mint alloy: Estimation of copper by volumetry and nickel by gravimetry
6) Analysis of hindalium: Estimation of aluminium and iron
7) Analysis of wood's alloy:
8) Analysis of solder sample:

SUGGESTED BOOKS

1. Quantitative Inorganic Analysis by A.I.Vogel.2nd edition .ELBS London.1985
2. A Text Book of Soil Chemical Analysis, P.R. Hesse CBS, new Delhi, 2002.
3. Practical Inorganic Chemistry, G. Marr and B.W. Rockett, Van Nostrand Reinhold Co. London 1972.
4. Quantitative Inorganic Analysis, Day and Underwood. 1985

OPEN ELECTIVE FOR NON-CHEMISTRY STUDENTS

C-304-MATERIAL SCIENCE AND NANOMATERIALS

52 Hours

UNIT-I

13h

Introduction

Introduction and definition of nanoparticles and nanomaterials, emergence of nanotechnology, Challenges of nanotechnology. Nanotechnology in relation to other branches of science.

Structure of solids: crystalline and non-crystalline. Types of common materials and advanced materials inorganic, organic, biological. Types of nanomaterials depending upon their properties: electronic, semiconductors, superconductors, superionic, magnetic, optic, opto-electronic, spintronics, lasers, photonics, ceramics, bioceramics, biomedical, biosensors, bioimagers, photocatalysts, quantum dots.

UNIT-II

13h

Preparation techniques

Principles of solid state synthesis-ceramic methods, solid solution and compound precursors, sol-gel, spray, pyrolysis, and combustion, hydrothermal, electrosynthesis.

Preparation of nanoscale materials: Precipitation, mechanical milling, colloidal routes, self assembly, chemical vapour deposition, sputtering, evaporation.

UNIT-III

13h

Characterization

X-rays, Spectroscopic - infrared, UV-Vis, Laser Raman, Photoluminescence, Diffussive reflectance spectroscopy, Electron Microscopic techniques (SEM, TEM), Thermal analysis, surface characteristics, light scattering methods, gas adsorption, magnetic susceptibility, conductivity, band gap calculations.

UNIT-IV

13h

Applications

Nanotechnology in modern technology in relation to electronic, biological, consumer and domestic applications. Energy related application: photo-volatile cells. Energy storage nanomaterials.

Sensors: Agriculture, health and medical, food, security.

Applied nanobiotechnology and nanobiomedical science drug delivery, drug targeting, biosensors, bioimaging, neutron capture therapy.

SUGGESTED BOOKS

1. Encylopedia of nanomaterials and nanotechnologies, H. S. Nalva.
2. Nanostructures materials: Processing, Properties and applications, C. C. Kouch, William Andrew publications, Newyork, 2002.
3. Introduction to nanotechnology, C. P. Poole Jr, F. J. Owens, 2nd edition, Wiley-India, Delhi, 2008.

4. Nanostructures and nanomaterials, G. Cao, Imperial College Press, University of Washington, USA, 2004.
5. Biomaterials, S. V. Bhat, 2nd edition, Narasa Publishing house, New Delhi, 2005.
6. Nanotechnology Fundamentals and applications, M. Karkare, I. K. international publishing house pvt. Ltd., Bangalore, 2008.
7. Nanomaterials: Synthesis, properties and applications, A. S. Edelstein, T. C. Cammarata, Inst. Of. Physics, UK, 1966.
8. Springer Handbook of Nanotechnology, B. Bhusan, 3rd edition, Springer-Verlag, 2009.
9. Chemistry of Nanomaterials: Synthesis, Properties and Applications, CNR Rao and T. Cheetham, Wiley & Sons, 2005.
10. Encyclopedia of Nanotechnology, Hari Singh Nalwa, American Scientific Publishers, 2004.

C-304: CHEMISTRY OF BIOMOLECULES

52 Hours

UNIT-I

Chemistry of plant products **6h**

Anthocyanins: Methods of isolation, basic structural features of coumarins, chromones, flavones and isoflavones. Structural elucidation of quercetin and wedelactone (synthesis not included).

Carotenoids: Methods of isolation; Structure elucidation of b-carotene; structural relationship of α, β and γ-carotenes.

Lipids **7h**

Introduction, isolation and properties of lipids. Oils and fats: definitions and significances of hydrogenation, iodine value, saponification value and auto-oxidation of oils and fats. Phospholipids: lecithins, cephalins and phosphatidyl serine. Sphingolipids: sphingosine, sphingomyelin and cerebrocides.

UNIT-II

Terpenoids, Steroids and Alkaloids **10h**

Terpenoids: Introduction, Biological importance, Nomenclature, Occurance and isolation; Isoprene rule; Structure and biosynthesis of monoterpenoids, sesquiterpenoids, diterpenoids and triterpenoids; Structures of camphene, pinenes, camphor, borneols.

Steroids: Sterols and Bile acids; Nomenclature, Basic skeleton, Diels hydrocarbon. Isolation, structure and structures of sterols and bile acids, stereochemistry at ring junctions. Structure and biological significance of Estrone, Progesterone, androsterone, testosterone; Photoproducts of ergpsterol- vitamins D.

Alkaloids: Definition, nomenclature, occurrence, isolation and classification. Study of general methods of structural elucidation, synthesis and biogenesis of papaverine..

Carbohydrates **6h**

Types of naturally occurring sugars. Deoxy sugars, amino sugars, branched chain sugars, methyl ethers and acid derivatives of sugars. General methods of structure and ring size determination with particular reference to maltose, lactose and sucrose.

Structure, degradation and biological functions of starch, cellulose and chitin.

UNIT-III

Amino acids, Peptides and Proteins **8h**

Classification, general methods of preparation, properties and reactions of amino acids. Peptide bond; nomenclature and classification of peptides; Proteins: biological importance, classification based on structure and composition. General idea of the peptide linkage and primary structure of proteins and its determination; Sanger and Edman methods; Denaturation and renaturation-thermal denaturation- aufinsens experiment with ribonuclease. Biosynthesis of peptides.

Vitamins **3h**

Biological importance and synthesis of Vit A, Vit. B_6, Vit C and Vit E (tocopherol).

UNIT-IV

Nucleic acids **8h**

Purine and pyrimidine bases. Structure of nucleosides and nucleotides. Methods of formation of internucleotide bonds (DCC, phosphotriester approach). Structure of DNA (Watson-Crick model) and RNAs. Biological importances of DNA and RNAs. Protein-nucleic acid interaction-chromatin and viral nulear capsid.

Prostaglandins **4h**

General study, nomenclature, classification, structure and biological role of PGE_1. PGE_2 and PGE_3.

SUGGESTED BOOKS

1. Biochemistry, J. David Rawn, Neil Pattuson publishers, North Carolina, (USA) 1989.
2. Organic Chemistry. Vol I and Vol II, I. L. Finar, 6th edn. ELBS & Longman (London), 1975.
3. Inroduction to Lipids, D. Chapman, McGraw-Hill, 1969.
4. Advanced general Organic Chemistry, S. K. Ghosh, DK and Allied publishers (UBS), Calcutta, 1998.
5. Text book o Biochemistry, E. S. West, W. R. Todd, H. S. Mason & J. T. Van Bugen, 4th Edn. Amerind publishing co. (New Delhi), 1974.

THIRD SEMESTER

INORGANIC CHEMISTRY SPECIALISATION
C-301 IC SOLID STATE CHEMISTRY

52 Hours

UNIT-I

Electronic structure of solids **7h**

Bonding in solids: Ionic, covalent, metallic and molecular solids

Free electron theory, Fermi sphere, Fermi-Dirac statistics, Ohm's law, limitations of the free electron theory

Electrons in a weak periodic potential (Independent electron model), energy levels in extended, repeat and reduced zone schemes

Electrical and Magnetic Properties of Solids **9h**

Metals: calculation of density of states, origin of resistivity, weak paramagnetism

Semiconductors: Intrinsic and extrinsic- p and n-types, Hall effect, Junctions and their applications- metal-metal, metal-semiconductor, semiconductor-semiconductor types and transistors.

Insulators- dielectric properties, piezo and inverse piezoelectric effects, ferroelectricity, ferroelectric transitions in $BaTiO_3$, ionic conductivity applications of band theory to TiO and NiO: Limitations of the Independent electron model, modeling electron correlation.

UNIT-II

Dynamics of Atoms in a Solid **4h**

Dispersion curves of an elastic structureless medium, Longitudinal and Transverse modes, Optical and Acoustic modes of a crystal, total vibrational energy of a crystal. Case study of calcite.

Defects in Solids **2h**

Point defects, Line defects and Plane defects, Stacking faults and grain boundaries

Superconductivity **4h**

Superconductivity, Meisner effect, Type I and type II superconductors, Features of superconductors, Frolich diagram, Cooper pairs, Theory of low temperature superconductivity, *Junctions using superconductors*

Phase Transition in Solids **2h**

Definitions, Classification of phase transitions, First and second order phase transitions: *Martensitic transition, order-disorder transitions and spinodal decomposition*

UNIT-III

Geometric Crystallography **5h**

Symmetry elements, Bravais lattices, Screw axes and glide planes, point groups, and space groups and nomenclature. Law of Interfacial angle (Euler's construction).

Diffraction theory and Single crystal X-ray diffraction **9h**

X-rays, Bragg's law, assignment of lines, diffraction pattern of a primitive cubic lattice, space group extinctions, Scaterring factor and structure factor, intensities from atomic positions for

BCC and FCC lattices; Ewald's sphere of reflection, Reciprocal Lattice concept, Electron density function, Fourier synthesis, Fourier transform of the structure factor, Phase problem and Patterson synthesis.

UNIT-IV

Experimental Methods **3h**

Rotation, Oscillation, Weissenberg and Precession methods. Debye-Scherrer method (Powder method), Determination of lattice parameters from these methods.

Electron diffraction **2h**

Experimental technique, Wierl equation, Radial-Distribution method**.**

Neutron diffraction **2h**

Principle and Theory, advantages and uses.

SUGGESTED BOOKS

1. Introduction to Solids, L. V. Azaroff, McGraw Hill Book Co., New York, 1960.
2. Solid State Physics, N. W. Ashcroft and N. D. Mermin, Holt Saunders International Ltd., New York (1976).
3. Physical Chemistry, G. M. Barrow, McGraw Hill (2nd ISE) (1966).
4. An Introduction to X-ray Crystallography, M. M. Woolfson, Cambridge University Press-Vikas Publishing House, New Delhi (1980).
5. Principles of the Solid State, H. V. Kheer, Wiley Eastern Ltd., New Delhi (1993).
6. Dynamics of Atoms in Crystals, W. Cochran, Edward Arnold, London, 1973. (pages 24-37)
7. Vibrational Spectroscopy of Solids, P.M.A. Sherwood, University Press, Cambridge, 1972. (pages: 1-45)
8. Phase Transitions, C.N.R. Rao and K.J. Rao, Cambridge University Press
9. X-ray Structure determination: A practical guide, George H Stout and Lyle H Jenson, Macmillan Publishing Co.Inc and Collier Macmillan Publishers

C - 302 ADVANCED ANALYTICAL TECHNIQUES

(Common to Inorganic and Analytical Chemistry)

52 Hours

UNIT-I

Optical Methods of Analysis

Atomic Absorption spectroscopy: 16h

absorption, emission, fluorescence phenomenon, principles and differences, Flame AAS, Instrumentation, different types of nebulizers, Nonflame techniques, GAAS, electrothermal vapourisers, graphite furnace, cold vapour AAS, radiation sources, HCL, EDL, TGL etc. detectors, photoemmissive cells, PMT, photodiodes, Interferences, spectral, chemical, matrix, background absorption, correction methods, deuterium arc, zeeman effect, Smith-Hieftje methos, single beam and double beam instruments, evaluation procedures, applications of AAS,

UNIT-II

Atomic Emission Spectroscopy: 8h

Emission-priciple, Inductively coupled plasma optical emission spectrometry, theory, ICP characteristics, sample introduction methods, tourch configuration and view modes, analytical performance.merits and limitations of AES over AAS, Detection limit, application to elemental analysis.

Microwave induced plasma systems in atomic spectrometry, principal processes, applications.

Mass spectrometry in the analysis of inorganic compounds-different techniques, applications.

Electroanalytical techniques-I 4h

Electrode Potential, Currents in Electrochemical cells, Potentiometric titrations. Electrogravimetry-faraday's laws of electrolysis, Coulometry, Coulometric titrations.

UNIT-III

Electroanalytical techniques-II 8h

Voltammetry- principle, DME-advantages,limitations, HydrodynamicVoltammetry, Cyclic voltammetry-priciple, conditions for reversible, quasi reversible and irreversible reactions Anodic stripping voltammetry-priciple and applications, Polarography, Pulse polarography, Amperometry-titrations, different titration curves,applications, numerical problems on all these techniques .

Thermal methods of analysis 7h

Principle, methodology and applications: thermogravimetric and differential thermal analysis, differential scanning calorimetry; Thermo-mechanical and dynamic mechanical analysis ; thermometric titrations. Thermal stability of polymers, applications, decomposition patterns, decomposition reactions-examples.

UNIT-IV

Analysis of Biomolecules 9h

Introduction, single biomolecule detection and characterization, Fluorescence, principle, factors influencing fluorescence, fluorescence based biosensors, fluoroimmunosensors,

Mass spectrometry-principle, sample preparation, probe tip, MALDIMASS, types of ion separation, instrumentation-types, applications in structural biology,
Application of NMR spectroscopy in the analysis of biomolecules,
Raman spectroscopy- phenomenon, merits and limitations, application to biomolecules,
Voltammetry in Vivo for chemical analysis of neurotransmitters in central nervous system

SUGGESTED BOOKS

1. Analytical Chemistry. Gary D Christian, 5th Edition, John – Wiley and Sons Inc., (1994)
2. Fundamentals of Analytical Chemistry.D. A. Skoog, D. M. West and F. J. Holler, 7th Edition, Saunders College Publishing (1996).
3. Instrumental methods of Analysis.H. H. Willard, L. L. Merrit, J. A. Dean and F. A. Set, CBS Publishers (1996).
4. Instrumental methods of Chemical Analysis, G. W. Ewing, 5th edition, McGraw-Hill, New York, 1988.
5. Electrochemical methods: A.J. Bard & l. R. Faulkner, 2nd edition, Wiley, New York, 2000.
6. Vogel's text book of Quantitative Chemical analysis 5th edition, Ed., Jeffery et. al ELBS/Longman, 1989
7. Encyclopedia of Analytical Chemistry: Ed. By R.A. Meyers Vol. 1 – 15, John Wiley, 2000.
8. Fundamentals of Instrumental Analysis, Skoog, D. M. West and F. J. Holler, 8th Edition, Saunders College Publishing (2004).

C-303 SPECTROSCOPY-II

(Common to Analytical, Inorganic and Physical Chemistry Students)

52Hours

UNIT-I

13h

Ultraviolet and Visible Spectroscopy

Classification of electronic transitions, Terminology, Substituent and solvent effects, UV spectral study of alkenes, polyenes, enones and aromatic compounds. Emprical rules for calculating lamda max.

Vibrational Spectroscopy

Sampling techniques, Group frequencies, factors affecting group frequencies, Bond order, Mass effect, Conjugation, Inductive, resonance, steric effects, intramolecular interactions. Application of IR in the study of H-bonding and tautomerism. Complimentarity of IR and Raman. Identification of the following organic compounds by IR: Alkanes, Alkenes, Alkynes, Aromatic compounds, Aldhydes, Ketones, Alcohols, Acids and its derivatives; Amines, Esters, Alkyl halides and Nitro compounds; Problems using UV and IR.

UNIT-II

13h

Nuclear Magnetic Resonance Spectroscopy

Introduction, Magnetic properties of nuclei-Resonance condition, Nuclear spin, population of nuclear spin levels and NMR isotopes, Relaxation methods, Instrumentation and sampling handling; Classical approach and FT-NMR.

Chemical shift, Factors influencing chemical shifts : electronegativity and electrostatic effects; Mechanism of shielding and deshielding in alkanes, alkyl halides, alkenes, aromatic compounds, carbonyl compounds and annulenes. Pascals triangle-low and high resolution, Reference compounds (internal and external reference compounds) Karplus Curve, Diamagnetic and Paramagnetic effects and Magnetic anisotropy. Equivalence of protons-chemical and magnetic equivalence; Spin systems: First order and second order coupling of AB systems, Simplification of complex spectra. Problems.

Spin-spin interactions: Homonuclear coupling interactions - AX, AX_2, AX_3, AMX, AB types. Vicinal, germinal and long range coupling-spin decoupling; Chemical shift reagents and deuterium exchange; Stereochemistry and hindered rotations. Temperature effects.

CIDNP, Nuclear Overhauser effect (NOE), Factors influencing coupling constants and Relative intensities.

UNIT-III

13h

^{13}C NMR Spectroscopy

Types of CMR spectra-undecoupled, proton decoupled, Off-resonance decoupled (SFORD); Selectively decoupled and gated decoupled spectra. ^{13}C chemical shifts of alkanes, alkyl halides, alkenes, alkynes, alcohols, ethers, carbonyl compounds and aromatic compounds; Factors affecting the chemical shifts. Applications of **13** C NMR spectroscopy in confirmation of structure and stereochemistry of organic molecules and in determining the reaction mechanism and dynamic processes of organic reactions – examples.

Mass Spectrometry-I

Basic principles - instrumentation ;Ion production : Soft ionization methods: Low energy electron ejection; Chemical ionization; Ionization of large molecules : Fast-atom bombardment (FAB), Plasma desorption (PD) and Matrix Assisted Laser Desorption/ionization (MALDI); Electrospray ionization (ESI); Pyrolysis; Exact mass measurements (high resolution spectra); Tandem mass spectrometry (MS/MS); Combined techniques;

UNIT-IV

Mass Spectrometry-II **13h**

Classification of mass spectrometers: Magnetic field deflection: magnetic field only (unit resolution) and double focusing (electrostatic field and magnetic field); High resolution; Quadrapole mass spectrometers: i. quadrupole mass filter and quadrupole ion storage (ion trap) Time of flight mass spectrometers; FT-ICR (ion cyclotron resonance spectrometers); MS/MS (tandem mass spectrometry).

Mass spectrum: Unit mass molecular ion and isotope peaks; High resolution molecular ion; recognition of the molecular ion peak; Use of molecular formula;

Fragmentation of alkanes, alkenes, alkyl halides, alcohols, aldehydes, ketones (cyclic and acyclic compounds), acids, esters, ethers, amines, nitro and halo compounds, peptides; Nitrogen rule; Factors affecting cleavage patters; McLafferty rearrangement;

Composite problems; Use of HRMS to determine exact molecular weight of compounds;

Application of UV, IR, NMR and mass methods in the structural elucidation of organic compounds

SUGGESTED BOOKS

1. Application of absorption spectroscopy to organic compounds, J. R. Dyer, Prentice-Hall, New Delhi, 1969.
2. Organic spectroscopy, P. Laszlo and P. Strang, Harper and Row, New York, 1971.
3. Organic spectroscopy, W. Kemp, ELBS London, 2000.
4. Spectrometric identification of organic compounds, sixth edition, R. M. Silverstien, and F. X. Webster, 2004.
5. Introduction to spectroscopy, 3rd Edition, D. L. Pavia, G. M. Laupman and G. S. Kriz, Harcourt college publishers,2001.
6. Interpretation of mass spectra, Fourth edition, F.W. McLafferty, F. Turecek, California, 1993.
7. Practical organic mass spectroscopy, 2nd edition, J R Chapman, John Wiley, NY, 1993,
8. The IR spectra of complex molecules, Vols.1 and 2, L J Bellamy, Chapman and halli, London,1975.
9. Spectroscopic techniquies for organic chemists, J W Cooper, John Wiley, NY, 1980.
10. Bimolecular NMR Spectroscopy, J N S Evans, Oxford univ. 1995.
11. Mass spectroscopy a foundation course. K Downard, RSC, Cambridge, 2004.
12. Instruemental methods of analysis, H. H. Willard, L. L. Merrit, J. A. Dean and F.A. Settle, CBS Publishers and Distributors, 1986.

C-304-[OPEN ELECTIVE, NON-CHEMISTRY PAPER]

THIRD SEMESTER

ORGANIC CHEMISTRY SPECIALISATION

C-301 OC: ORGANIC REACTION MECHANISMS

52 Hours

UNIT-I

Aliphatic nucleophilic and electrophilic substitution reactions **10h**

Nucleophilic substitution reactions:

Substitution at allylic carbon (allylic rearrangement), at a trigonal carbon (hydrolysis of esters and amides, use of DCC in the formation of anhydrides), substitution at a vinylic carbon. Neighboring group participation and $S_N i$ reactions.

Electrophilic substitution reactions:

SE2, SE1 and SEi mechanisms. Hydrogen exchange, migration of double bonds, α-halogenation of aldehydes, ketones and acids. Aliphatic diazonium coupling, nitrosation at carbon bearing active hydrogens, diazo transfer reaction, carbene and nitrene insertion, decarboxylation of aliphatic acids, haloform reaction, Haller-Bauer reaction.

UNIT-II

Free-radical chemistry **10h**

Generation of free-radicals: Thermal homolysis of peroxides, peresters and azo compounds, photochemical methods.

Free radical reactions: Free-radical mechanisms in general. Free-radical substitution mechanisms. Mechanisms at an aromatic substrate. Neighboring group assistance in free-radical reactions. Reactivity for aliphatic substrates, reactivity at a bridgehead, reactivity in aromatic substrates, reactivity in the attacking radical. Halogenation at an alkyl carbon and an allylic carbon, hydroxylation at an aliphatic carbon, hydroxylation at an aromatic carbon, oxidation of aldehydes to carboxylic acids, formation of hydroperoxides and peroxides, Gomberg-Bachmann reaction, Meerwein arylation, Sandmeyer reaction, Kolbe reaction and Hunsdiecker reaction.

UNIT-III

Photochemistry **11h**

Physical and Chemical processes, Jablonski diagram. Photosensitization, quantum efficiency, quantum and chemical yields.

Photochemistry of functional groups:

i) *Olefins*: *Cis-trans* isomerism, [2 + 2]-cycloaddition, rearrangements. Reaction of conjugated olefins; di-π-methane rearrangements (including oxa- and aza- di-π-methane rearrangements).

ii) *Ketones*: Excited state of C=O. Norrish type-I and type-II cleavages. Paterno-Buchi reaction. α,β-unsaturated ketones. [2+2] addition. Rearrangement of cyclohexadienones (application in the synthesis of some important natural products).

iii) *Aromatic compounds*: Photorearrangement of benzene and its derivatives, cycloaddition of benzene.

iv) *Photochemical oxidations and reductions*: Cycloaddition of singlet molecular oxygen {[2+2], [4+2]-additions}. Oxidative coupling of aromatic compounds, photoreduction by hydrogen abstraction.

Pericyclic reactions-I **6h**

Molecular orbital symmetry, Woodward-Hoffmann correlation diagrams. FMO and PMO approaches. Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl system. Electrocyclic reactions: conrotatory and disrotatory motions, 4n, 4n+2 and allyl systems. Cycloadditions: antarafacial and suprafacial additions, $[_{\pi}m_s + _{\pi}n_a]$ and $[_{\pi}m_s + _{\pi}n_s]$-cycloadditions. $[_{\omega}2_a + _{\pi}2_s]$ and $[_{\pi}4_s + _{\omega}2_s]$-cheletropic reactions.

UNIT-IV

Pericyclic reactions-II **5h**

Regio, enantio and Endo selectivities in Diels-Alder reactions. Hetero Diels-Alder reaction. Sigmatropic rearrangements: suprafacial and antarafacial shifts of H, sigmatropic shifts involving carbon moieties. [*i, j*]- sigmatropic rearrangements (including Walk, Claisen, Cope, oxy and aza-Cope rearrangements).

Biochemical mechanisms **10h**

Introduction. The mechanistic role of the following in living systems.

i). Thiamine pyrophosphate (TPP) in decarboxylation of α-ketoacids and in the formation of α-ketols.
ii). Pyridoxal phosphate (PLP) in transamination, decarboxylation, dealdolisation and elimination reactions of amino acids.
iii). Lipoic acid in the transfer of acyl group reactions.
iv). Coenzyme A (CoASH) in the transfer of acyl group.
v). Biotin and
vi). Vitamin KH_2 coenzyme in carboxylation reactions.
vii).Tetrahydrofolic acid (H_4F) in one-carbon transfer reactions.
viii).Vitamin B_{12} coenzymes in molecular rearrangement reactions and in the synthesis of methionine and methane.
ix). Nicotinamide and
x). Flavin coenzymes in biological redox reactions

SUGGESTED BOOKS

1. Advanced Organic Chemistry – Reactions, Mechanism and Structure, Jerry March, John Wiley (2008).
2. Understanding organic reaction mechanisms, A. Jacob, Cambridge Univ. Press, 1997.
3. Introduction to organic chemistry A. Streitweiser, Jr and C. H. Heathcock, Macmillan, 1985.
4. Physical and mechanistic organic chemistry, R.A.Y. Jones, 1st Edn. Cambridge Univ. Press, 1979.
5. Mechanisms of molecular migrations, Vols I and II, B. S. Thiagarajan, 1st Edn. Pergamon Press, Oxford, 1979.
6. P. J. Garratt in Comprehensive organic chemistry, D. Barton and W. D. Ollis, 1st Edn. Pergamon Press, Oxford, 1979.
7. Radicals in organic synthesis, B. Giese, Pergamon Press, 1986.

8. Stereoelectronic effects in organic chemistry, P. Deslongchamps, 1st Edn. Pergamon Press, 1983.
9. Frontier orbitals and organic chemical reactions, Ian Fleming, John Wiley, 1980.
10. Molecular orbital theory for organic chemistry, A. Streitweiser, 1st Ed. Wiley & Sons, NY, 1969.
11. Organic photochemistry, J. M. Coxon and B. Halton, 1st Edn, Cambridge Univ. Press, London, 1974.
12. Orbital symmetry, R. E. Lehr and A. P. Marchand, Academic Press, 1972.
13. Molecular reactions and photochemistry, C. H. Deputy and D. S. Chapman, 1st Edn. Prentice-hall India, New Delhi, 1972.
14. Stereochemistry of Organic Compounds: Principles and Applications, D Nasipuri, New-Age International, (1999).
15. Biochemistry, G. Zubey, Macmillan, NY, 1998.
16. Biochemistry, D. Voet and J. G. Voet, John Wiley & Sons, 1998.
17. Principles of Biochemistry, A. L. Lehninger, D. L. Nelson & M. M. Cox, 2nd Edn. Worth Publishers, NY, 2005.

C-302 OC CHEMISTRY OF NATURAL PRODUCTS

52 Hours

UNIT-I

Terpenoids and Carotenoids **12h**

Classification, nomenclature, occurrence and isolation. Isoprene rules.
Stereochemistry of citral, farnesol, limonene, 1,8-cineole, menthols and borneols.
Correlation of configurations of terpenoids.
Structure elucidation of camphene, α-pinene, β-caryophyllene, α-santonin and gibberrillic acid.
Synthesis and biosynthesis of the following:
Linalool, α-terpineol, fenchone, eudesmol, abietic acid.
Commercial synthesis of camphor.
Biosynthesis of squalene and cyclisation of squalene into α-lanosterol and friedelene.
Carotenoids: Methods of isolation. Structural relationship of α-, β- and γ-carotenes. Structure elucidation and synthesis of β-carotene.

UNIT-II

Alkaloids **12h**

Definition, nomenclature, occurrence, isolation, classification, General methods of structure elucidation. Synthesis and biosynthesis of the following alkaloids:
Ephedrine, hygrine, coniine and cocaine.
Cinchona alkaloids: Cinchonine and quinine.
Opioid alkaloids: Morphine, codeine, thebiene and heroin.
Structure elucidation and synthesis of papaverine, reserpine and ergotamine.
Photochemical synthesis of Nuciferine, coradyline and tylophorine.

UNIT-III

Porphyrins and vitamin B_{12} **7h**

Structure elucidation and synthesis of haemin, chlorophyll-a and vitamin-B_{12} (synthesis of Vitamin-B_{12} from cobyric acid).

Nucleic acids **8h**

Introduction, components of nucleic acids, nucleosides, nucleotides and oligonucleotides.
Structure elucidation and synthesis of nucleosides and nucleotides.
Chemical synthesis of oligonucleotides: Protecting groups for hydroxy group in sugar, amino group in the base and phosphate functions. Methods of formation of internucleotide bonds: DCC, phosphodiester approach, phosphotriester approach, phosphite triester and phosphoramidite methods. Solid phase synthesis of oligonucleotides.

UNIT-IV

Prostaglandins **7h**

Introduction, nomenclature, classification and biological role of prostaglandins. Structure elucidation and stereochemistry of PGE_1, PGE_2 and PGE_3. Synthesis of PGE_1 and PGE_2 by Corey's and Stork's approaches. Synthesis of PGE_3 by Upjohn's approach. Synthesis of prostacyclin I_2 and thromboxane B_2. Biosynthesis of prostaglandins.

Insect pheromones **6h**

Introduction, classification. Pheromones in pest control.

Syntheses of (one synthesis should be stereoselective synthesis)

i) Grandisol (component of boll weevil pheromone)
ii) Farenal (trail pheromone of pharaoh's ants)
iii) Brevicomin (pheromone from *Dendroitis brevicomis)*
iv) (+)- Disparlure (gypsy moth sex pheromone).
v) 3,11-Dimethy1-2-nonacosanone (pheromone of German cockroaches).
vi) Bombykol (sex pheromone of silkworm moth).
vii) Multistriatin (Elm bark beetle sex pheromone).

SUGGESTED BOOKS

1. Natural products: Their chemistry and biological significance-J. Mann, R. S. Davidson, J. B. Hobbs, D. V. Banthorpe & J. B. Harborne, Longman, UK, 1994.
2. Terpenes, J. Verghese, Tata McGraw-Hill, New Delhi, 1982.
3. Chemistry of terpenes and terpenoids, A. Newman, Academic Press, London, 1975.
4. Handbook of naturally occurring compounds Vol. II: Terpenes, T. K. Davon, A. I. Scott, Academic Press, NY, 1972.
5. Natural products chemistry Vol. I & II, K. Nakanishi, T. Goso, S. Ito, S. Natori & S. Nozoe, Academic Press, NY, 1974.
6. Total synthesis of natural products Vol. I & VI, Apsimon, John Wiley, NY, 1973-1981.
7. Organic chemistry Vol.II, I. L. Finar, 6th Edn. Longman, 1992.
8. Chemistry of natural products Vol. I & II, O. P. Aggarwal, Goel Publishing House, 6th Edn. 1982.
9. Total synthesis of natural products: The chiral approach Vol.III, S. Hanessian Pergamon Press, 1983.
10. Total synthesis of steroids, Akhaun & Titov, Jerusalem, 1969.
11. Medicinal natural products: A biosynthetic approach, P. M. Dewick. John Wiley, Chichester, 1997.
12. The colours of life: An introduction to the chemistry of porphyrins and related compounds, L. R. Milgrom, Wiley Chichester, 1995.
13. Interpretation of the UV spectra of natural products, A.I. Scott, Pergamon Press, Oxford, 1964.
14. Spectral data of natural products Vol. I- K.Yamaguchi, Elsevier Publishing Co, London, 1970.
15. Chemistry of natural products: A unified approach, N. R. Krishnaswamy, University Press, India, 1999.

C-303: OC: ORGANIC SPECTROSCOPY

52 hours

UNIT-I

Ultraviolet and visible spectroscopy **6h**

Classification of elecgronic transitions, Terminology, Substituent and solvent effects, UV spectral study of alkenes, polyenes, enones and aromatic compounds. Empirical rules for calculating λ_{max}.

Vibrational Spectroscopy: spectroscopy **9h**

Sampling techniques, Group frequencies, factors affecting group frequencies, Bond order, Mass effect, Conjugation, Inductive, resonance, steric effects. Intramolecular interactions. Applicaton of IR in the stuy of H-bonding, stereoisomerism and tautomerisam. Complimentarity of IR and Raman. Identification of the following organic compounds by IR: Alkanes, Alkenes, Alkynes,
Aromatic compounds, Aldehydes, Ketones, Alcohols, Acids, Acid chlorides,
Amides, Amines, Esters, Halides, Nitro compounds, etc., problems using UV and IR.

UNIT-II

Nuclear magnetic resonance spectroscopy-I **13h**

Introduction, Magnetic properties of nuclei- Resonance condition. Nuclear spin, population of nuclear spin levels and NMR isotopes, Relaxation methods. Insturmetnation and sample handling, FT-NMR.

Chemical shift. Mechanism of shielding and deshielding in Alkanes, Alkyl halides, Alkenes, Aromatic compounds, Carbonyl compounds and Annulenes. Pascal's triangle-low and high resolution, spectrum of ethnaol. Karplus Curve, Diamagnetic and paramagnetic effects and magnetic anisotropy. Equivalence of protons-chemical and magnetic equivalence. Spin-systems: First order and second order coupling of AB systems, Simplifications of complex spectras.

Problems.

Spin-spin interactions: AX,AX_2, AX_3, AMX,AB types. Vicinal, geminal and long range coupling-Spin decoupling. Chemical shift reagents and deuterium exchange. Stereochemistry and hindered rotations. Temperature effects.

UNIT-III

Nuclear magnetic resonance spectroscopy-II **12h**

CIDNP, Nuclear Overhauser effect (NOE). Factors influencing coupling constants and Relative intensities. Protons attached to elements other than carbon.

^{13}C NMR Spectroscopy: Range and factors affecting chemical shifts of alkanes, alkyl halides, alkenes, alcohols, ethers, alkynes, carbonyl compounds and aromatics..

Multiple resonance spectroscopy: Introduction to 2D-techniques: DEPT, COSY, HETCOR, and INADEQUATE.

Explanation of the principle, applications to structure elucidation and stereochemistry of simple organic molecules.

Dynamic NMR.

NMR spectroscopy of other nuclei with spin I = ½. Introduction to ^{15}N, ^{19}F, ^{29}Si and ^{31}P NMR spectroscopies. Chemical shift values for ^{15}N, ^{19}F, ^{29}Si and ^{31}P containing compounds.

UNIT-IV

Mass spectrometry and Composite Prooblems: 7h

Basic principles-instrumentation – ion production-ion analysis-magnetic sector instruments Quadrapole mass spectrometers. Time of flight mass spectrometers-ion cyclotron resonance spectrometers- Mass spectrum-molecular ion-types of ions in mass spectra and effects of isotopes on mass spectra. Methods of ionization, EI, FAB mass and MALDI methods. Fragmentation of Alkanes, Alkenes, alkyl halides, alcohols, aldehydes, ketones, acids, esters, ethers, amines, nitro and halo compounds peptides, Nitrogen rule, Factors affecting cleavage patterns. MeLafferty and MeLafferty +1 rearrangment. Determination of molecular formula. Composite problems.

Use of HRMS to determine exact molecular formulae of compounds.

Application of UV, IR, NMR and MS methods and chemical reactions in the structure elucidation of organic compounds. **5h**

SUGGESTED BOOKS

1. Applications of absorption spectroscopy to organic compounds, J. R. Dyer, Prentice-Hall, New Delhi, 1969.
2. Organic spectroscopy, P. Laszlo and P. Stang, Harper & Row, New York, 1971.
3. Organic spectroscopy, W. Kemp, ELBS London, 2000.
4. Spectrometric identification of organic compounds, R. M. Silverstien, and W. P. Weber, 2005.
5. Introduction to spectroscopy, 3rd Edn., D. L. Pavia, G. M. Laupman and G. S. Kriz, Harcourt College Publishers, 2001.
6. Organic mass spectroscopy, K. R. Dass & E. P. James, IBH New Delhi, 1976.
7. Interpretation of organic mass spectra, F. W. McLafferty, W. A. Benjamin, London, 1973.
8. Practical Organic Mass Spectroscopy, 2nd Edn. J R Chapman, John Wiley, NY, 1993.
9. The IR Spectra of complex molecules, Vols. I and II, L J Bellamy, Chapman and Hall, London, 1975.
10. Spectroscopic techniques for Organic Chemists, J W Cooper, John Wiley, NY, 1980.
11. Biomolecular NMR Spectroscopy, J N S Evans, Oxford Univ. 1995.
12. Mass spectrometry a foundation course, K Downard, RSC, Cambridge, 2004.
13. Mass spectrometry of organic compounds, H. Budzkiewicz, Djerassi C. and D. H. Williams, Holden-Day New York, 1975.
14. Modern NMR techniques and their Applications, Ed. A I Popov, Marcel Deckker, 1991.
15. Modern structural theory of organic compounds, L. N. Ferguson, Prentice-Hall, New Delhi, 1973.
16. Instrumental methods of analysis, H. H. Willard, L. L. Merrit, J. A. Dean and F.A. Settle, CBSPublishers and Distributors, 1986.
17. Fundamentals of molecular spectroscopy, 4th edn., C. N. Banwell and E. M. McCash,Tata McGraw-Hill, New Delhi, 1999.

C-304-[OPEN ELECTIVE, NON-CHEMISTRY PAPER]

THIRD SEMESTER

PHYSICAL CHEMISTRY SPECIALISATION

C-301 PC: SOLID STATE CHEMISTRY

52 Hours

UNIT-I

13h

Electronic structure of solids.

Free electron theory of solids, results of free electron theory; limitations and success of free electron theory, Fermi distribution, Fermi sphere, volume of Fermi sphere, expression for energy levels in a solid, density of states, expression for the number of energy levels in a Fermi sphere.

Electrical properties of Solids

Electronic conductivity: Ohm's law, derivation of Ohm's law, Hall Effect, Band theory, Zone theory, Brillion zones, K-space, k-vector, Significance of k-vector, Semiconductors: Energy bands in a semi conductor, temperature dependence of conductivity in metals and semi conductors, intrinsic and extrinsic semiconductors, Insulators; properties, Piezo and inverse Piezo electric effect. Pyroelectricity, Magnetic properties

UNIT-II

13h

Crystal Defects

Point defects; Schottky, Frenkel and interstitial, line defects and plane defects.

Heat Capacity of Solids

Definition, Theories of heat capacity of solids: Dulong-petit, Einstein's theory, Debye Theory. Problems and their solution

Superconductivity

Features of Superconductors, BCS theory, Meisner effect, Type I and Type II superconductors, Frolich diagram, Cooper pairs.

UNIT-III

13h

Phase transitions in Solids:

Definition, Classification of phase transitions: First and second order phase transitions. Martensitic transitions, Order-disorder transitions, Spinodal decompostions **5h**

Symmetry and structure of solids

Symmetry elements in solids; Screw axis and glide planes, Hermann-Maguin notations, Crystal systems, Bravais lattices, space lattice, point groups, and space groups, Law of interfacial angel (Euler's equation). Number of rotation axes in solids

UNIT-IV

13h

X-Ray Diffraction

X-rays, Bragg's law, scattering of x-rays by solids; Scattering factor, structure factor, intensity of scattering, Electron density. Reciprocal Density concept, Braggs Law in Reciprocal space, Fourier Synthesis, Fourier Transform of structure factor.

Electron diffraction

Principle and scattering of electron beam, Wierl equation, radial distribution technique.

Neutron diffraction

Scattering of neutron beam by solids, Scattering factor, advantages of neutron diffraction.

2h

SUGGESTED BOOKS

1. Introduction to solids, L.V. Azoroff, McGraw Hill Book Co., New York, 1960.
2. Solids State Physics, N.W. Ashcroft and N. D. Mermin, Holt Saunders International Ltd., New York (1976).
3. Physical Chemistry, G. M. Barrow, McGraw Hill (2nd ISE) (1966).
4. An Introduction to X-ray Crystallography, M. M. Woolfson, Cambridge University Press-Vikas Publishing House, New Delhi (1980).
5. Principles of the solid State, H.V.kheere, Wiley Eastern Ltd., New Delhi (1993).
6. X-Ray structure determination: A practical guide, George H Sout and Lyle H Jenson, Macmillan Publishing Co.Inc and Collier Macmillan Publishers.
7. Crystal Structure analysis for Chemists and biologists, J.P. Glusker, M.Lewis and M .Ross, Wiley-VCH (1994).

C-302 PC QUANTUM CHEMISTRY & SURFACE CHEMISTRY

52 Hours

UNIT-I

QUANTUM CHEMISTRY-I: Theories of valence **13h**

Introductory aspects: Linear and non-linear variation functions. Secular equations. Coulombic, exchange, normalization and overlap integrals. Secular determinants. Molecular orbital (MO) theory, LCAO-MO approximation, application to Hydrogen molecule ion (H_2^+), energy levels of H_2^+, bonding and antibonding molecular orbitals, electron distribution, potential energy diagrams, comparison of theoretical and experimental values of energy. Valence bond (VB) theory of H_2molecule, the Heitler-London method, energy levels, energy distribution. Various modifications of the Heitler-London wave function.

Comparison of MO and VB theories. Ionic terms, fractional ionic characters and its importance,Equivalence of simple MO and VB methodsion-covalent resonance and configuration interaction. LCAO treatment of diatomic molecules, LCAO forms of simple wave function and molecular orbitals. Notations of molecular orbitals: full notation, Mulliken notation. MO configuration of homo- and hetero-nuclear diatomic molecules. Molecular electric terms. Bond order, stability and magnetic behavior of molecules from M.O. diagrams, isoelectronic systems. Correlation diagrams, non-crossing rule.

UNIT-II

QUANTUM CHEMISTRY-II: **13h**

The HF-SCF-LCAO method. Directed valence, hybridization, Expressions for hybrid orbitals in terms of wave functions of s and p orbitals and explanation of directed valences of sp, sp^2, and sp^3 hybrid orbitals. Hybridization involving d-orbitals,Localized and non-localized molecular orbitals in polyatomicmolecules(H_2O).

Huckel molecular orbital theory: Outline of the method including assumptions. Application to ethylene, allylrdical, cyclopropenyl radical, butadiene, cyclobutadiene, bicyclobutadiene and benzene. Calculation of delocalization energy, charge density, π-mobile bond order and free valence.

UNIT-III

SURFACE CHEMISTRY-I

A. Review of adsorption curves, Adsorption-desorption, Adsorption forces, Heat of adsorption- Types, Measurements of heat of adsorption (Calorimetric and Clausius Clapeyron method), Measurement of adsorption isotherms, (Volumetric and Gravimetric methods), Determination of entropy of adsorption, Electrostatic adsorption, adsorption indicators and their applications. Volcanic curves. Applications of adsorption. **6h**

B. Adsorption kinetics: Kinetics of chemisorption (Hertz-Knudsen equation), Chemisorptive bond, Competitive adsorption, Mechanism of some catalyzed surface reactions, Kinetic effects of surface heterogeneity, Kinetic effects of interactions, Potential energy curves for adsorption, Transition state theory of surface reactions, Rates of desorption, Kinetics of bimolecular surface reactions, Langmuir-Hinshelwood Mechanism, Langmuir-Rideal mechanism, Rideal-Eley mechanism and their comparison. **7h**

UNIT-IV

SURFACE CHEMISTRY-II

C. Adsorption theories: Polanyi's potential theory and Polarization theory. Hysteresis Of adsorption. **3h**

D. Surface structure: Surface mobility, Surface heterogeneity, Surface area and its determination by point-B method, Harkins-Jura method, Radioactive tracer method and Benton and White method. Importance of surface area. Examination of surfaces by Interferometer method, Scanning electron microscopy (SEM), Low energy electron diffraction method (LEED method), Field Emission spectroscopy, Auger electron spectroscopy(AES), STM, and TEM. **10h**

SUGGESTED BOOKS

1. Molecular Quantum mechanics, P.W. Atkins and R.S. Friedman, Oxford university press (1997).
2. Introductory Quantum Chemistry by A. K. Chandra, Tata McGraw Hill (1994).
3. Quantum Chemistry by R.K. Prasad, 3rdEdn, New Age International (2006).
4. Quantum Chemistry by Ira N. Levine, Prentice Hall, New Jersey (1991).
5. Quantum Chemistry by Donald A McQuarrie, Viva Books Pvt. Ltd.New Delhi, India, Published in arrangement with Unversity Science books, Sausalito, CA, USA (2003).
6. Physical chemistry of surfaces by A. W. Adamson, Interscience Publishers Inc., New York (1967).
7. Surface Chemistry: Theory and Applications by J.J Bikertman, Academic Press, New York (1972).
8. Chemical Kinetics by K.J Laidler, 3rdEdn., Harper International Edn., (1987).
9. Text Book of Physical Chemistry by S. Glasstone, McMillan India Ltd.2ndEdn., (1986).
10. Physical chemistry, `R J Silbey, R A Alberty and M G bawendiEdn, Willey (2009).
11. Physics at surfaces, A Zangwill, Cambridge university Press (1988).
12. Surface crystallography, L J Clarke, Wiley-Interscience (1985).

C-303 SPECTROSCOPY-II

(Common to Analytical, Inorganic and Physical Chemistry Students)

52Hours

UNIT-I

13h

Ultraviolet and Visible Spectroscopy

Classification of electronic transitions, Terminology, Substituent and solvent effects, UV spectral study of alkenes, polyenes, enones and aromatic compounds. Emprical rules for calculating lamda max.

Vibrational Spectroscopy

Sampling techniques, Group frequencies, factors affecting group frequencies, Bond order, Mass effect, Conjugation, Inductive, resonance, steric effects, intramolecular interactions. Application of IR in the study of H-bonding and tautomerism. Complimentarity of IR and Raman. Identification of the following organic compounds by IR: Alkanes, Alkenes, Alkynes, Aromatic compounds, Aldhydes, Ketones, Alcohols, Acids and its derivatives; Amines, Esters, Alkyl halides and Nitro compounds; Problems using UV and IR.

UNIT-II

13h

Nuclear Magnetic Resonance Spectroscopy

Introduction, Magnetic properties of nuclei-Resonance condition, Nuclear spin, population of nuclear spin levels and NMR isotopes, Relaxation methods, Instrumentation and sampling handling; Classical approach and FT-NMR.

Chemical shift, Factors influencing chemical shifts : electronegativity and electrostatic effects; Mechanism of shielding and deshielding in alkanes, alkyl halides, alkenes, aromatic compounds, carbonyl compounds and annulenes. Pascals triangle-low and high resolution, Reference compounds (internal and external reference compounds) Karplus Curve, Diamagnetic and Paramagnetic effects and Magnetic anisotropy. Equivalence of protons-chemical and magnetic equivalence; Spin systems: First order and second order coupling of AB systems, Simplification of complex spectra. Problems.

Spin-spin interactions: Homonuclear coupling interactions - AX, AX_2, AX_3, AMX, AB types. Vicinal, germinal and long range coupling-spin decoupling; Chemical shift reagents and deuterium exchange; Stereochemistry and hindered rotations. Temperature effects.

CIDNP, Nuclear Overhauser effect (NOE), Factors influencing coupling constants and Relative intensities.

UNIT-III

13h

^{13}C NMR Spectroscopy

Types of CMR spectra-undecoupled, proton decoupled, Off-resonance decoupled (SFORD); Selectively decoupled and gated decoupled spectra. ^{13}C chemical shifts of alkanes, alkyl halides, alkenes, alkynes, alcohols, ethers, carbonyl compounds and aromatic compounds; Factors affecting the chemical shifts. Applications of **13** C NMR spectroscopy in confirmation of structure and stereochemistry of organic molecules and in determining the reaction mechanism and dynamic processes of organic reactions – examples.

Mass Spectrometry-I

Basic principles - instrumentation ;Ion production : Soft ionization methods: Low energy electron ejection; Chemical ionization; Ionization of large molecules : Fast-atom bombardment (FAB), Plasma desorption (PD) and Matrix Assisted Laser Desorption/ionization (MALDI); Electrospray ionization (ESI); Pyrolysis; Exact mass measurements (high resolution spectra); Tandem mass spectrometry (MS/MS); Combined techniques;

UNIT-IV

Mass Spectrometry-II **13h**

Classification of mass spectrometers: Magnetic field deflection: magnetic field only (unit resolution) and double focusing (electrostatic field and magnetic field); High resolution; Quadrapole mass spectrometers: i. quadrupole mass filter and quadrupole ion storage (ion trap) Time of flight mass spectrometers; FT-ICR (ion cyclotron resonance spectrometers); MS/MS (tandem mass spectrometry).

Mass spectrum: Unit mass molecular ion and isotope peaks; High resolution molecular ion; recognition of the molecular ion peak; Use of molecular formula;

Fragmentation of alkanes, alkenes, alkyl halides, alcohols, aldehydes, ketones (cyclic and acyclic compounds), acids, esters, ethers, amines, nitro and halo compounds, peptides; Nitrogen rule; Factors affecting cleavage patters; McLafferty rearrangement;

Composite problems; Use of HRMS to determine exact molecular weight of compounds;

Application of UV, IR, NMR and mass methods in the structural elucidation of organic compounds

SUGGESTED BOOKS

1. Application of absorption spectroscopy to organic compounds, J. R. Dyer, Prentice-Hall, New Delhi, 1969.
2. Organic spectroscopy, P. Laszlo and P. Strang, Harper and Row, New York, 1971.
3. Organic spectroscopy, W. Kemp, ELBS London, 2000.
4. Spectrometric identification of organic compounds, sixth edition, R. M. Silverstien, and F. X. Webster, 2004.
5. Introduction to spectroscopy, 3rd Edition, D. L. Pavia, G. M. Laupman and G. S. Kriz, Harcourt college publishers, 2001.
6. Interpretation of mass spectra, Fourth edition, F.W. McLafferty, F. Turecek, California, 1993.
7. Practical organic mass spectroscopy, 2nd edition, J R Chapman, John Wiley, NY, 1993,
8. The IR spectra of complex molecules, Vols.1 and 2, L J Bellamy, Chapman and halli, London, 1975.
9. Spectroscopic techniquies for organic chemists, J W Cooper, John Wiley, NY, 1980.
10. Bimolecular NMR Spectroscopy, J N S Evans, Oxford univ. 1995.
11. Mass spectroscopy a foundation course. K Downard, RSC, Cambridge, 2004.
12. Instruemental methods of analysis, H. H. Willard, L. L. Merrit, J. A. Dean and F.A. Settle, CBS Publishers and Distributors, 1986.

C-304-[OPEN ELECTIVE, NON-CHEMISTRY PAPER]

C 305, 306, 307 and 308 Practicals
Inorganic, Organic, Physical and Analytical Chemistry practicals (I Sem Syllabus)
(4 days a week, 4 hours a day)

FOURTH SEMESTER

ANALYTICAL CHEMISTRY SPECIALISATION

C-401 AC: SOLID STATE AND RADIOANALYTICAL CHEMISTRY

52 Hours

UNIT-I

13h

Geometric Crystallography: Symmetry elements, Bravais lattices, Screw axes and glide planes, point groups, and space groups and nomenclature. Law of Interfacial angle (Euler's construction).

Experimental Methods: Rotation, Oscillation, Weissenberg and Precession methods, Debye-Scherrer method (Powder method), Determination of lattice parameters from these methods.

Electron diffraction: Experimental technique, Wierl equation, Radial-Distribution method**.**

Neutron diffraction: Principle and theory; advantages and uses.

UNIT-II

13 h

Diffraction theory and Single crystal X-ray diffraction

X-rays, Bragg's law, assignment of lines, diffraction pattern of a primitive cubic lattice, space group extinctions, Scaterring factor and structure factor, intensities from atomic positions for BCC and FCC lattices; Ewald's sphere of reflection, Reciprocal Lattice concept, Electron density function, Fourier synthesis, Fourier transform of the structure factor, Phase problem and Patterson synthesis.

UNIT-III

14 h

Nuclear properties and models: Subatomic particles: protons, neutrons, quarks, spin and magnetic properties of nucleons, electrical quadrupole moment of nuclides, nuclear parity, nuclear statistics, nuclear forces and interactions. Nuclear models: liquid drop, shell model, Fermi gas model, collective model and optical model.

Radiation Chemistry: Interaction of matter with radiation, radiation dosimetry-units and measurements using chemical dosimeters, radiolysis of water, the hydrated electron-recipitation and properties, free radical generation, radiation damage to solids-effects of radiation on metals, alloys, semiconductors, insulators and catalysts.

UNIT-IV

12 h

Applications of Radioactivity: Synthesis of various useful isotopes, use of isotopes in the elucidation of reaction mechanism, structure determination, kinetics of exchange reactions, measurement of physical constants including the diffusion constants, radio analysis-isotope dilution techniques, NAA, PGNAA, neutron absoptiometry and age determination, radio isotopes in field of medicine.

SUGGESTED BOOKS

1. Introduction to Solids, L.V.Azaroff, McGraw Hill Book Co., New York, 1960.
2. An Introduction to X-ray Crystallography, M.M.Woolfson, Cambridge University Press-Vikas Publishing House,New Delhi(1980)
3.Physical Chemistry, G. M. Barrow, McGraw Hill (2nd ISE) (1966).
4. X-ray Structure determination: A Practical Guide, George H Stout and Lyle H Jenson,Macmillan Publishing Co.Inc and Macmillan Publishers
5. Essentials of Nuclear Chemistry, H.J. Arnikar Wiley Eastern Ltd. New Delhi
6. Instrumental method of analysis.H.H.Willard, L.L.Merrit, J.A.Den and F.A.Settle, CBS publishers and distributors, 1986.
7.Principles of Instrumental Analysis, D.A Skoog, F.J. Holler and T.A. Nieman, Thomson 5th Edn. 2004
8. Instrumental methods of Chemical Analysis, G.W. Ewing McGraw Hill 2004

C-402 AC ENVIRONMENTAL AND BIOANALYTICAL CHEMISTRY

52 Hours

UNIT-I

13 h

Environmental Chemistry: Introduction: Environmental chemistry, environmental segments, classification of environmental pollution.

Air Pollution: Introduction, Air pollutants, Primary pollutants – Sources (CO, NO_x, HC, SO_2, particulates). Particulates – Sources (Inorganic and organic particulate matters). Effects on: Humans, materials, vegetation and animals.
Air quality standards, Sampling, monitoring and analysis: CO by gas chromatography, NO_x by Spectrophotometric method using sulphanilamide and NEDA, SO_2 by pararosaniline (PRA), H_2S by colorimetric using ethylene blue, hydrocarbons by chemiluminescence, Control of air pollution: Control of particulate matter and gaseous pollutants

Radioactive Pollution

Introduction, Sources, Radiation from natural and manmade activities, Radioactive effects on human and plants, Storage and disposal of radioactive waste, Detection and monitoring of radioactive pollutants.

UNIT-II

13 h

Water Pollution: Introduction, Sources, Water pollutants classification: Organic pollutants – Pesticides, insecticides, detergents. Inorganic pollutants, Sediments, Radioactive materials and Thermal pollutants. Drinking water supplies, Trace elements in water. COD, BOD, TOC-definitions. Monitoring techniques and methods: Determination of pH, conductance, dissolved oxygen by Winkler's method, nitrate/nitrite by diazo coupling, chloride by Mohrs and Volhard's method, and fluoride by Alizarin Visual method, Water contamination with cyanide, sulfide, sulphate, phosphate and total hardness.Analysis of Arsenic by Atomic absorption spectroscopy (AAS), cadmium and mercury by dithizone method, chromium by diphenyl carbazide method, lead by polarographic method.Water pollution control and management.

Soil Analysis

Introduction, Origin and nature of soil, Sources of soil pollution and explanation in brief, Purpose of soil analysis, Techniques for the analysis of soil - Lime Potentials: Moisture measurement by gravimetric method, pH using calomel glass electrode method, total nitrogen by kjeldhal method, determination of nitrate-nitrogen by Bratton and Marshal method, determination of potassium and sodium by Flame photometry, calcium by EDTA titration , organic matter by combustion, total sulphur by oxidation as sulphate.

UNIT-III

13 h

Food Analysis: Sampling, Preparation and storage of samples, Estimation of moisture, ash, crude protein, crude fat, sugars, nitrogen, crude fibre, starch in food.

Polyphenols: Extraction, detection and analysis, characterization and spectral identifications of anthocyanins and anthocyanidins. Estimation of Tannins.

Vitamins: Estimation of Vitamin-C (Ascorbic acid), Thiamine, Riboflavin, Folic acid Minerals: Preparation of sample, Estimation of calcium, Magnesium, phosphorus, iron, potassium, sodium, copper, tin, zinc, lead, arsenic, mercury.

Lipids**:** General composition of edible oils, Physical and chemical characteristics. Composition and structure of free fatty acids. Test for the presence of specific oils: Ground nut oil, Sesame oil, cottonseed oil, linseed oil, argemone oil, presence of mineral oil, Fatty acid analysis. Estimation of fatty acid composition, tests for stability of fats.

UNIT-IV

13 h

Analysis of Drugs: Drug design: Characteristics of an ideal drug molecule, mechanism of drug interaction, Antibiotics, classification and structure, mode of action, Theory and assay of Aspirin(titrimetry), methyldopa (nonaqueoustitrimetry) , Analgin(iodimetry), chloral hydrate (argentiometry), cholesterol (gravimetry) , hydrocortisone acetate (tetrazolium assay).

Clinical Chemistry: Composition of blood, collection, and preservation of samples-anticoagulants, protein precipitants. Interpretation and Clinical analysis of Blood glucose(glucose oxidase methods), proteins, blood urea (Nesslerisation method). Lipids, Calcium, phosphorus, phosphatases, iodine, iron, copper, Sulfur, Magnesium, Chloride, sodium and potassium.

SUGGESTED BOOKS

1. Dr. H. Kaur, Environmental Chemistry (2010)
2. Khopkar. S. M, Environmental pollution, monitoring and control, IIT Mumbai (2004)
3. Asim K. Das, Environmental Chemistry with Green Chemistry (2010)
4. P. R. Hesse , A text book of Soil Chemical Analysis (2002)
5. A. K. De, Environmental Chemistry (7th edition), Uttarpara West Bengal (2010)
6. N. Manivasakam, Physico chemical examination of water, sewage and industrial effluents (6th edition 2010)
7.Hand book of Analysis and Quality control for fruit and vegetable products. S Ranganna, Tata McGraw-Hill Publishing Co. Ltd, Second Edition
8. Pharmaceutical Drug Analysis. AshutoshKar, New Age International Publishers
9. Practical Clinical Biochemistry, Harold Varley, Fourth Edition
10. Food Analysis, A G Woodman, McGraw-Hill
11. Principles of Medicinal ChemistryVol 1, Dr. S S, Kadam, Dr. K R Mahadic, Dr. K G Bothara, Niraliprakashan

C 403: CHEMISTRY OF MATERIALS

(Common to Inorganic and Analytical Chemistry)

52 Hours

UNIT-I

14 h

Preparative Techniques: Principles of solid state synthesis- ceramic methods, solid solution and compound precursors (nitrates, carbonates, hydroxides, cyanides and organometallics), sol-gel, spray pyrolysis, combustion, hydrothermal, electrosynthetic

New Materials

Fullerenes and fullerides – structure, synthesis, functionalization approaches, conducting properties of fullerides.applications.

NASICON and alumina – structure and conducting properties.

High-T_c Oxides - structure, perovskite A & B, structure and synthesis of La,Sr and Ba cuprates, applications..

Conducting polymers - PA, PPP, PPS, PPY-mechanism of conduction and applications.

UNIT-II

12 h

Nanomaterials: Classification types of carbon nano tubes synthesis, functionalization charecterization and applications.

Principles of self-assembly: surfactant solutions, importance of non-covalent forces, the hydrophobic effect, co-operativity, statistical mechanics of one-dimensional self-assembly.

Preparation of nanoscale materials: Precipitation, mechanical milling, colloidal routes, self assembly: chemical vapour depostition, sputtering, evaporation.

Synthesis, characterization and applications of nanoparticles, nano wires and nanotubes. Elemental nanoparticles: Pure, Gold, Silicon, Silver ,Cobalt, Oxide nanoparticles: Silica, Zinc oxide, Iron oxide, Alumina.

UNIT-III

14 h

Intercalation Compounds: Intercalation reactions **-** layered structure-graphite interlayer compounds (GILC), staging of graphite, TaS_2, Microporous materials – zeolites and zeolitic materials, $AlPO_4$- $GaPO_4$.

Fibres and Composites

Synthetic inorganic polymers- zirconia and other fibre Classification, microscopic composites, dispersion strengthned, particle reinforced,Fibre-glass reinforced composites, metal-matrix, plastic-matrix composites, hybrid composites.

UNIT-IV

12 h

Amorphous Materials: Crystalline versus amorphous solids, glass formation, Prepararion techniques- meltspinning, sputtering, ion implantation, Structural models of amorphous materials, Properties of metglasses - mechanical, electronic and magnetic properties.

Liquid Crystals: Mesomorphic behaviour, classification, examples - thermotropic and lyotropic liquid crystals Calamitic, nematic phase A, B, smectic phase, chiral nematic phase and optical Properties of liquid crystals. Applications with special reference to display systems

SUGGESTED BOOKS

1. Encyclopedia of Nanomaterials and Nanotechnology Hari Singh Nalva
2. Nanostructured Materials: Processing, Properites and Applications, ed. C.C.Koch, Willaim Andrew Publishing, New York, 2002.
3. Nanomaterials: Synthesis, properties and applications, Ed. By A.S.Edelstein and R.C. Cammarata, Inst. of Physics, UK 1966.
4. Science of Engineering Materials, C.M. Srivastava and C. Srinivasan, Wiley-Eastern Ltd. (1991).
5. Solid State Chemistry and its Applications , A.R. West, John Wiley & Sons.(1989).
6. Material Science and Engineering. W.D. Callister , John Wiley and Sons Inc. (1985).
7. Nanotubes and Nano wires CNR Rao, & A Govindaraj, RSC, London 2005.
8. NANO: The essentials T. Pradeep, McGraw-Hill, 2008.
9. Liquid Crystals, Nature's delicate phase of matter, Peter J Collings, Princeton University Press,2002
10. Nanochemistry, A chemical approach to Nanomaterials, Geoffrey A Ozin and Andre C Arsenault, RSC, 2006.

C-404 SPECTROSCOPY – III

(Common to Analytical, Inorganic and Physical Chemistry)

52 Hours

UNIT-I

Vibrational spectroscopy **9h**

Vibrational spectra of diatomic, linear and bent triatomic, AB_3, AB_4, AB_5 and AB_6 molecules, spectra of metal complexes: Ammine, amido, Nitro, Nitrito, lattice water, aquo and hydroxo, carbonato, nitrato, sulphato and other acido complexes, cyano and nitrile complexes, cyanato and thiocyanato complexes, mono and multinuclear carbonyl complexes, nitrosyls, phosphines and arsines, ambidentate ligands, ethylenediamine and diketonato complexes

Raman spectroscopy **4h**

Resonance Raman Spectroscopy, Nonlinear Raman effects-Stimulated, hyper and inverse types, Lasers and their use in Raman spectroscopy

Photoacoustic spectroscopy: Basic description and applications **2h**

UNIT-II

Photoelectron spectroscopy **8h**

Basic principles- photoelectric effect, Koopman's theorem, XPS and UPS, spin-orbit coupling in core level spectra, applications of core level spectra-ESCA, chemical shift, Valence level spectra- n, σ and π bands, Auger electron spectroscopy and applications, Electron energy loss spectroscopy- basic principles and applications

Applications to the study of solids

NMR spectroscopy of inorganic molecules **8h**

Proton NMR spectra of metal hydride complexes

NMR spectra of nuclei other than hydrogen: ^{19}F, ^{31}P, ^{11}B NMR spectra of simple compounds, Proton/hydride interactions with ^{103}Rh, ^{183}W, ^{195}Pt and ^{207}Pb in metal complexes/organometallic compounds, Solid State NMR.

UNIT-III

Electron spin resonance spectroscopy **10h**

Basic principles, the position of ESR absorption, significance of 'g' factor, determination of 'g'factor. Electron-nucleus coupling (Hyperfine splitting). ESR spectrometer, electron-electron coupling, double resonance in ESR, ENDOR, ELDOR. Interpretation of ESR spectra and structure elucidation of organic radicals using ESR spectroscopy. Spin density and Mc Connell relationship. Spin polarization for atoms and transition metal ions, spin-orbit coupling and significance of g-tensors, zero/non-zero field splitting, Kramer's degeneracy, application to transition metal complexes (having one to five unpaired electrons) including biological molecules and inorganic free radicals such as PH_4, F_2 and BH_3.

UNIT-IV

Mossbauer spectroscopy **5h**

Basic principles, isomer shift, quadrupole splitting and magnetic hyperfine interactions, application to the study of bonding and structures of Fe^{2+} and Fe^{3+} compounds, Sn^{2+} and Sn^{4+} compounds

NQR spectroscopy **4h**

NQR isotopes, electric field gradients, Nuclear Quadrupole coupling constants, Experimental techniques and applications

X-ray absorption spectroscopy **2h**

Near edge measurements and EXAFS

SUGGESTED BOOKS

1. Physical methods in Inorganic Chemistry, R.S. Drago, Affiliated East West Press Pvt. Ltd., New Delhi (1965).
2. Infrared spectra of Inorganic and Coordination Compounds, K. Nakamoto, Wiley Interscience, New York (1970).
3. Vibrational Spectroscopy: Theory and Applications, D.N. Sathyanarayana, New Age International Publishers, New Delhi (2000).
4. Electronic Absorption Spectroscopy and Related Techniques, D.N. Sathyanarayana, Universities Press, Bangalore (2001).

ANALYTICAL CHEMISTRY PRACTICALS
(2 days a week, 4 hours a day)

C- 405 Analytical Chemistry Practicals – V

1. Estimation of nitrite using chloramines T
2. Estimation of copper using salicylaldoxime
3. Estimation of sulphate as benzidine sulphate
4. Estimation of metal acetates using perchloric acid in glacial acetic acid medium
5. Separation of metal ions by paper chromatography/TLC
6. Estimation of Iron III by solvent Extraction
7. AAS Estimation of Cu, Fe and Ni
8. Flame photometric estimation of K, Na from soil extract sample
9. Preparation and characterization of a metal complex by IR spectroscopy
10. Synthesis of zeolites and measurement of surface acidity
11. Synthesis of spinels/pervoskites and their characterization by XRD studies
12. Determination of pka of amino acids by potentiometric titration
13. Determination of dissociation constant of phosphoric acid by potentiometric titration
14. Determination of stability constant of copper-ethylenediamine complex by potentiometry
15. Spectrophotometric determination of metal-ligand ratio in Iron-phenanthroline complex by Job's method
16. Spectrophotometric determination of pKa value of an indicator
17. Spectrophotometric determination of uranyl ion by solvent extraction
18. Estimation of copper by electrogravimetric method
19. Polarographic analysis, identification and estimation of metal ions(pb^{2+}, Cd^{2+}, Zn^{2+})
20. Cyclic voltammetry of a standard redox couple(ferricyanide-ferrocyanide couple)
21. Determination of fluoride in drinking water by spectrophotometry(Zr-Alizarin method)

SUGGESTED BOOKS

1. Text book of Quantitative Inorganic Analysis by A.I. Vogel,ELBS(1978)
2. Advanced Physicochemical Experiments by Rose, Isaac Pitman(1964)
3. Polarographic methods of analysis by Meites, L. Intersciences Publishers, Inc. NeYork,(1955)
4. Findlay's Practical Physical Chemistry by Levitt, Longmann's(1966)
5. Experimental Physical chemistry by J B Yadav, Goel Pub. House,(1981)
6. Methods of Soil analysis Part I & II, C.A. Black et al(Ed) American Society of Agronomy, Inc. (1965).

C - 406 Analytical Chemistry Practicals - VI

1. Estimation of total nitrogen content by kjeldal method
2. Separation of lipids by thin layer Chromatography
3. Separation of amino acids by thin layer chromatography
4. Separation of proteins by gel electrophoresis
5. Estimation of fat in milk
6. Estimation of rancidity in a sample of butter
7. Estimation of nitrite/nitrate in water samples
8. Estimation of nicotine in tobacco

9. Estimation of a common drug(paraacetamol)
10. Estimation of COD of a water sample9industrial effluent)
11. Estimation of lead in water samples
12. Extraction of caffeine from tea leaves, characterization by IR,
13. Estimation of glucose in serum
14. Estimation of Cholesterol in serum
15. Estimation of blood urea nitrogen
16. Estimation of protein in food samples
17. Estimation of Vitamin A in food samples
18. Estimation of alkaline phosphatase
19. Analysis of calcium and magnesium in milk
20. Estimation of nitrite nitrogen by diazocoupling reaction colorimetrically

SUGGESTED BOOKS

1. Experiments in Environmental chemistry, P.D.Vowels and D.W.Connel, Pergamon(1980).
2. Vogel's Practical Organic Chemistry, Ed.A.J.Hannaford, ELBS London (1978).
3. Practical Clinical Biochemistry , H.Varley and Anold Heinmann(1978)
4. An introduction to practical Biochemistry, David Plummer,Tata McGraw Hill(1979)
5. Laboratory Manual in Biochemistry, J. Jayaraman,Wiley Eastern(1981)
6. Chromatography, C. G. Sharma

ANALYTICAL CHEMISTRY

C-407: PROJECT WORK
(8 Hours PER WEEK)

FOURTH SEMESTER
INORGANIOC CHEMISTRY SPECIALISATION

C-401 IC: ORGANOMETALLIC CHEMISTRY AND CATALYSIS

52 Hours

UNIT-I

Organometallic complexes- Stability and decomposition pathways, classification of ligands, nomenclature of organometallic complexes, 16 and 18 electron rules. Electron counting-covalent and ionic models.

Synthesis, structure, bonding and reactivity of the following organotransition metal complexes: Carbenes, carbynes, alkenes, alkynes, allyl moieties, butadiene, cyclobutadiene, cyclopentadiene, arenes, cycloheptadienyl moieties and cyclooctatetraene moieties. Ring slippage reactions, cyclometallation reaction. **13h**

UNIT-II

Organometallic compounds of main group elements- General trends, structure and bonding in Li and Al alkyls.

Fluxional behaviour in organometallic complexes: Fluxionality and dynamic equilibria in complexes containing CO, η^2-olefin η^3-allyl and dienyl complexes.

Organometallic compounds in organic synthesis: Green rules, synthesis and use of Zinc dialkyls, Collman's reagent, organomercuric and chromium carbonyls in organic synthesis, Heck reaction, hydrozirconation. **13h**

UNIT-III

A. Isoelectronic and isolobal analogy.

B. Catalysis- Basic principles, industrial requirements of catalysts. Homogeneous catalysis: Hydrogenation, asymmetric hydrogenation; hydrosilation- Chalk-Harrod mechanism: hydrocyanation- synthesis of buta-1,3-diene; hydroformylation- Cobalt and modified catalysts, Rh catalysts. **13h**

UNIT-IV

Wacker process- acetaldehyde from ethylene; Monsanto acetic acid process, cativa process, Tennessee Eastmann process- Acetic anhydride from methyl acetate.Olefin metathesis; water gas shift reaction; Oligomerization- Shell High Olefin process; alkene isomerisation. Fischer Tropsch Process; Ziegler Natta Polymerization- syndiotactic, isotactic polymers, living polymerization; ammonia synthesis; Anchored catalysis- merits, polymer and metal oxides as supports; catalytic converters. **13h**

SUGGESTED BOOKS

1. Organometallic Chemistry; R. C. Mehrotra and A. Singh; New age international, 2nd edition, 2000.
2. The organometallic chemistry of transition metals; R. H. Crabtee; John Wiley, 3rd edition, 2001.
3. Organometallic Chemistry, ch. Elschewbroich and Slazer, VCH, 2nd edition 1992.
4. Organometallics; Vol 1 & 2; M. Bochmann, Oxford Chemistry Primers, Oxford University Press, 1994.
5. Catalytic chemistry; B. C. Gates; John Wiley and sons, 1992.
6. Applied Organometallic chemistry and catalysis; Robin whyman, Oxford University Primers, 2001.
7. Basic Organometallic chemistry; B. D. Gupta and A. J. Elias, University Press, 2010.
8. Heterogeneous catalysis; D. K. Chakraborty and B. Viswanathan, New Age International, 2000.

C-402-IC: REACTION MECHANISMS AND BIOINORGANIC CHEMISTRY

52 Hours

UNIT-I

Reaction mechanism- Labile, inert, stable and unstable complexes, classification of mechanisms- energy profile of reactions having different mechanisms.
Substitution in square planar complexes- factors affecting substitution, trans-effect, theories of trans-effect, application of trans-effect in the synthesis of complexes.
Mechanism of ligand substitution in octahedral complexes- kinetics, factors affecting substitution in octahedral complexes: Leaving group, chelate and metal effects. Acid-Base catalysis: Acid catalysed aquation and anation reactions, base hydrolysis, conjugate base hydrolysis, stereochemistry of octahedral substitution, application of ligand substitution reactions for the synthesis of octahedral complexes. **13h**

UNIT-II

A. Electron transfer reactions, complementary and non-complementary, outer sphere electro transfer- Marcus equation, Inner sphere electron transfer- one and two electron transfer, use of electron transfer reactions for the synthesis of complexes.
B. Oxidative addition, reductive elimination, isomerisation, migratory insertion reactions.
C. Metal ligand interactions with DNA. Metal ion deficiency and treatment (Fe, Zn, Cu, Mn); toxicity of Fe, Cu, Heavy metals- As, Hg, Pb and Cd; detoxification; chelation therapy; metal complexes as anticancer and antiarthritic drugs. Biological roles of Ca: Binding sites of Ca^{2+} in proteins, importance of Ca^{2+} in muscle contraction and in blood clotting process. **13h**

UNIT-III

Na^+/K^+ transport across cell membranes, ionophores, crown ethers, Na^+/K^+ pump. Iron storage and transfer- ferritin, transferrin and siderophores.
Oxygen transport and oxygen uptake proteins- transport and storage of dioxygen; Heme proteins and oxygen uptake, structure and functions of haemoglobin and myoglobin, dioxygen binding, Bohr effect, Hill equation, role of distal and proximal histidine; Model complexes for dioxygen binding, non- porphyrin systems- hemerythrin and hemocyanin.
Photosynthesis and nitrogen fixation: Nitrogenase: structural aspects and functions, abiological nitrogen fixation. Photosynthesis: Chlorophyll- structural features, role of Mg^{2+}- Z scheme of photosynthesis-PSI and PSII. **13h**

UNIT-IV

Structure and functions of metalloproteins in electron transfer process- Cytochromes, ferridoxines- 2Fe-2S, Rieske centers, high potential iron proteins; 4Fe-4S, 3Fe-4S, 8Fe-8S and rubredoxin. Mitochondrial flow of electrons from NADH to oxygen, cytochrome C, Cytochrome C oxidase.
Metalloenzymes: Structure and reactivity- Zinc enzymes: carboxypeptidase, carbonic anhydrase, alcoholdehydrogenase. Cu enzyme: superoxide dismutase. Mo enzyme: Xanthine oxidase, nitrate reductase. Fe enzymes: catalase, peroxidise and cytochrome P-450. Vitamin B_{12}: Coenzyme: B_{12r}, B_{12s}, biochemical functions of cobalamins; Biomethylation, mutase activity. **13h**

SUGGESTED BOOKS

1. Inorganic and organometallic reaction mechanism; J. D. Atwood; Brooks/cole publication co. (1985).
2. Reaction mechanism of inorganic and organometallic systems; J. B. Jordon, Oxford University Press 2nd edition, 1998.
3. Inorganic Chemistry, 3rd Edition; Gary. L. Miessler and Donald . A. Tarr (2007).
4. Inorganic Chemistry; K. F. Purcell and J. C. Kotz, Saunders company, 1977.
5. Bio-inorganic chemistry, I. Bertini, H. B. Gray, S. J. Lippard and J. S. Valentine, Viva Books Pvt. Ltd 1998
6. Bioinorganic Chemistry; Asim. K. Das; Books and allied (p) Ltd., 2007.
7. Principles of Bioinorganic Chemistry; S. J. Lippard and J. M. Berg; Panima Pub. Corporation 1997.

C 403: CHEMISTRY OF MATERIALS

(Common to Inorganic and Analytical Chemistry)

52 Hours

UNIT-I

14 h

Preparative Techniques: Principles of solid state synthesis- ceramic methods, solid solution and compound precursors (nitrates, carbonates, hydroxides, cyanides and organometallics), sol-gel, spray pyrolysis, combustion, hydrothermal, electrosynthetic

New Materials

Fullerenes and fullerides – structure, synthesis, functionalization approaches, conducting properties of fullerides.applications.

NASICON and alumina – structure and conducting properties.

High-T_c Oxides - structure, perovskite A & B, structure and synthesis of La,Sr and Ba cuprates, applications..

Conducting polymers - PA, PPP, PPS, PPY-mechanism of conduction and applications.

UNIT-II

12 h

Nanomaterials: Classification types of carbon nano tubes synthesis, functionalization charecterization and applications.

Principles of self-assembly: surfactant solutions, importance of non-covalent forces, the hydrophobic effect, co-operativity, statistical mechanics of one-dimensional self-assembly.

Preparation of nanoscale materials: Precipitation, mechanical milling, colloidal routes, self assembly: chemical vapour depostition, sputtering, evaporation.

Synthesis, characterization and applications of nanoparticles, nano wires and nanotubes. Elemental nanoparticles: Pure, Gold, Silicon, Silver ,Cobalt, Oxide nanoparticles: Silica, Zinc oxide, Iron oxide, Alumina.

UNIT-III

14 h

Intercalation Compounds: Intercalation reactions **-** layered structure-graphite interlayer compounds (GILC), staging of graphite, TaS_2, Microporous materials – zeolites and zeolitic materials, $AlPO_4$- $GaPO_4$.

Fibres and Composites

Synthetic inorganic polymers- zirconia and other fibre Classification, microscopic composites, dispersion strengthned, particle reinforced,Fibre-glass reinforced composites, metal-matrix, plastic-matrix composites, hybrid composites.

UNIT-IV

12 h

Amorphous Materials: Crystalline versus amorphous solids, glass formation, Prepararion techniques- meltspinning, sputtering, ion implantation, Structural models of amorphous materials, Properties of metglasses - mechanical, electronic and magnetic properties.

Liquid Crystals: Mesomorphic behaviour, classification, examples - thermotropic and lyotropic liquid crystals Calamitic, nematic phase A, B, smectic phase, chiral nematic phase and optical Properties of liquid crystals. Applications with special reference to display systems

SUGGESTED BOOKS

1. Encyclopedia of Nanomaterials and Nanotechnology Hari Singh Nalva
2. Nanostructured Materials: Processing, Properites and Applications, ed. C.C.Koch, Willaim Andrew Publishing, New York, 2002.
3. Nanomaterials: Synthesis, properties and applications, Ed. By A.S.Edelstein and R.C. Cammarata, Inst. of Physics, UK 1966.
4. Science of Engineering Materials, C.M. Srivastava and C. Srinivasan, Wiley-Eastern Ltd. (1991).
5. Solid State Chemistry and its Applications , A.R. West, John Wiley & Sons.(1989).
6. Material Science and Engineering. W.D. Callister , John Wiley and Sons Inc. (1985).
7. Nanotubes and Nano wires CNR Rao, & A Govindaraj, RSC, London 2005.
8. NANO: The essentials T. Pradeep, McGraw-Hill, 2008.
9. Liquid Crystals, Nature's delicate phase of matter, Peter J Collings, Princeton University Press,2002
10. Nanochemistry, A chemical approach to Nanomaterials, Geoffrey A Ozin and Andre C Arsenault, RSC, 2006.

C-404 SPECTROSCOPY – III

(Common to Analytical, Inorganic and Physical Chemistry)

52 Hours

UNIT-I

Vibrational spectroscopy **9h**

Vibrational spectra of diatomic, linear and bent triatomic, AB_3, AB_4, AB_5 and AB_6 molecules, spectra of metal complexes: Ammine, amido, Nitro, Nitrito, lattice water, aquo and hydroxo, carbonato, nitrato, sulphato and other acido complexes, cyano and nitrile complexes, cyanato and thiocyanato complexes, mono and multinuclear carbonyl complexes, nitrosyls, phosphines and arsines, ambidentate ligands, ethylenediamine and diketonato complexes

Raman spectroscopy **4h**

Resonance Raman Spectroscopy, Nonlinear Raman effects-Stimulated, hyper and inverse types, Lasers and their use in Raman spectroscopy

Photoacoustic spectroscopy: Basic description and applications **2h**

UNIT-II

Photoelectron spectroscopy **8h**

Basic principles- photoelectric effect, Koopman's theorem, XPS and UPS, spin-orbit coupling in core level spectra, applications of core level spectra-ESCA, chemical shift, Valence level spectra- n, σ and π bands, Auger electron spectroscopy and applications, Electron energy loss spectroscopy- basic principles and applications

Applications to the study of solids

NMR spectroscopy of inorganic molecules **8h**

Proton NMR spectra of metal hydride complexes

NMR spectra of nuclei other than hydrogen: ^{19}F, ^{31}P, ^{11}B NMR spectra of simple compounds, Proton/hydride interactions with ^{103}Rh, ^{183}W, ^{195}Pt and ^{207}Pb in metal complexes/organometallic compounds, Solid State NMR.

UNIT-III

Electron spin resonance spectroscopy **10h**

Basic principles, the position of ESR absorption, significance of 'g' factor, determination of 'g'factor. Electron-nucleus coupling (Hyperfine splitting). ESR spectrometer, electron-electron coupling, double resonance in ESR, ENDOR, ELDOR. Interpretation of ESR spectra and structure elucidation of organic radicals using ESR spectroscopy. Spin density and Mc Connell relationship. Spin polarization for atoms and transition metal ions, spin-orbit coupling and significance of g-tensors, zero/non-zero field splitting, Kramer's degeneracy, application to transition metal complexes (having one to five unpaired electrons) including biological molecules and inorganic free radicals such as PH_4, F_2 and BH_3.

UNIT-IV

Mossbauer spectroscopy **5h**

Basic principles, isomer shift, quadrupole splitting and magnetic hyperfine interactions, application to the study of bonding and structures of Fe^{2+} and Fe^{3+} compounds, Sn^{2+} and Sn^{4+} compounds

NQR spectroscopy **4h**

NQR isotopes, electric field gradients, Nuclear Quadrupole coupling constants, Experimental techniques and applications

X-ray absorption spectroscopy **2h**

Near edge measurements and EXAFS

SUGGESTED BOOKS

1. Physical methods in Inorganic Chemistry, R.S. Drago, Affiliated East West Press Pvt. Ltd., New Delhi (1965).
2. Infrared spectra of Inorganic and Coordination Compounds, K. Nakamoto, Wiley Interscience, New York (1970).
3. Vibrational Spectroscopy: Theory and Applications, D.N. Sathyanarayana, New Age International Publishers, New Delhi (2000).
4. Electronic Absorption Spectroscopy and Related Techniques, D.N. Sathyanarayana, Universities Press, Bangalore (2001).

INORGANIC CHEMISTRY PRACTICALS
(2 days a week, 4 hours a day)

C-405 Inorganic Chemistry Practicals- V

1. Determination of percentage purity of nitrite.
2. Estimation of sulphate by EDTA.
3. Estimation of Cu as Copper Salicyldoximate.
4. Microvolumetric estimation of chloride.
5. Analysis of Wood's alloy.
6. Analysis of $Co(NH_3)_6Cl_3$.
   i. Analysis of Cobalt volumetrically.
   ii. Estimation of NH_3 by Kjeldahl's method.
   iii. Estimation of Cl^- by gravimetric method as AgCl.
   iv. Molar absorption spectrum of $Co(NH_3)_6Cl_3$.
   v. Molar conductance of the complex.
7. Determination of magnetic susceptibility of $HgCo(SCN)_4$.
8. Preparation and analysis of $Pb(Ch_3COO)_4$ (non-aqueous reaction).
9. Preparation and IR spectral studies of pentamminenitrocobalt(III)chloride and corresponding nitrito complex.
10. Paper chromatographic separation of Co^{2+}, Ni^{2+}, Cu^{2+} and Zn^{2+} ions.

C-406 Inorganic Chemistry Practicals- VI

1. Flame photometric determination of Na^+ and K^+.
2. Determination of the stability constant of ferrisalicylate complex spectrophotometrically.
3. Colorimetric estimation of Ni.
4. Colorimetric estimation of Fe (1, 10-phenanthroline, SCN^- method).
5. Determination of conductivity of 1:1, 1:2 and 1:3 complexes.
6. Determination of Cu spectrophotometrically.
7. Estimation of Cu by electrogravimetry.
8. Non-aqueous titrations- Estimation of metal-acetate using perchloric acid in glacial acetic acid medium.
9. Spectrophotometric determination of metal-ligand ratio in Fe(1, 10-phenanthroline) complex using Job's method.
10. Spectrophotometric determination of Cr and Mn in Cr and Mn mixtures.

SUGGESTED BOOKS:

1. A text book of Quantitative Analysis; A. I. Vogel; ELBS, 1962.
2. Practical Inorganic Chemistry, G. Marr and B. W. Rockett, Von Nostrand Reinhold Co., London (1972).
3. Experimental Inorganic Chemistry; G. Palmer, Cambridge University Press, 1954.
4. Hand Book of preparative inorganic chemistry, Vols I and II; G. Brauer, Academic Press, 1963.
5. Non- aqueous titrations; W. Huber; Academic Press, 1967.
6. Experimental Methods in inorganic chemistry; T. Tanaka and S. L. Suib, Prentice Hall, 1999.
7. Experiments in Chemistry; D. V. Jahagirdar, Himalayan Pub House, 2003.

INORGANIC CHEMISTRY

C-407: PROJECT WORK
(8 Hours PER WEEK)

FOURTH SEMESTER
ORGANIC CHEMISTRY SPECIALIZATION

C-401: OC: ORGANOMETALLIC AND HETEROCYCLIC CHEMISTRY

52 Hours

UNIT-I

Organometallic Compounds in Organic Synthesis-I

Chemistry of Organotransition metal complexes:
General introduction. 18- and 16-Electron rules. General rules.
Complexation and De-complexation Reactions: s-Bonded systems including h1 ligands. p-Bonded systems involving dihapto to octahapto ligands such as- olefins, acetylenes, allyl moieties, butadiene, cyclobutadiene, arenes, cyclopenta, cyclohexa and cycloheptadienyl moieties; cyclohepta, cyclooctatrienes, and cyclooctatetraene moieties. **4h**
Use of organotransition metal complexes as protecting and stabilizing groups: Protection of olefins, acetylenes and dienes. Stabilization of cyclobutadines and norbornadienones.
Organometallics as electrophiles and nucleophiles: Nucleophilic addition to h2, h5 and h6 complexes. Electrophilic addition to h4, h6 and carbene complexes. **3h**
Organometallics in coupling and cyclization reactions: Coupling and cyclization of organic nucleophiles with olefins (including Heck reaction), and coupling of olefins with acetylenes (including Felkin's reaction). **3h**
Organometallics in isomerization, oxidation and reduction reactions: Isomerization of olefins, allylic alcohols and allylic ethers. Oxidation of olefins (including Wacker's process and epoxidation) and reduction of olefins and α,β-unsaturated compounds (including Wilkinson's reaction). **4h**

UNIT-II

Organometallic Compounds in Organic Synthesis-II

Carbonylation reactions:
Use of zirconium complexes in the synthesis of esters, acids, aldehydes or acyl halides from alkyl halides and in the hydroformylation of olefins and dienes.
Use of iron complexes for the insertion of CO group into organic molecules such as dienes, alkyl halides, and vinyl epoxides.
Use of cobalt complexes in the synthesis of ketones from epoxides, lactones from allylic alcohols and in the hydroformylation of olefins.
Use of palladium complexes for the carbonylation of alkyl halides, dienes and allenes. **4h**

Application of the following organometallics in Organic Synthesis:
Organozincs: Preparation, reaction with compounds containing acidic protons, reaction with C-C multiple bonds, trans-metallation, addition reactions of zinc reagents with carbonyl compounds. Simmons Smith, and Reformatsky reaction.
Organolithiums: Preparation. Deprotonation reactions, nucleophilic addition reactions, reactions with imines, nitriles and isonitriles.
Organocopper reagents: (Gilman reagents-lithium dialkyl cuprates): Preparation, reactions with alkyl, allyl, vinyl, benzyl and aryl halides, aldehydes, ketones (including a,b-unsaturated carbonyl compounds) and epoxides. **4h**

Organoseleniums: preparation. Use of organoseleniums in the synthesis of alkenes fromalkyl halides, α,β -unsaturated carbonyl compounds from carbonyl compounds.
Organotelluriums: Debromination of vic-dibromides, deoxygenation of epoxides, oxidation of hydroquinone and synthesis of biaryls.
Organoaluminiums: Preparation, hydroalumination and carboalumination of alkenes. Nucleophillic addition reactions with carbonyl compounds and Hydrocyanation. Preparation of alkenyldialkylalanes and their reactions. **4h**

UNIT-III

Organometallic Compounds in Organic Synthesis-III
Organosilicons: Introduction, preparation and general reactions of trialkylsilyl halides. Peterson olefination.
Organotins: Preparation and reactions of tri-*n*-butyltin hydride, Barton decarboxylation and Barton- McCombie reaction.
Organocerates: Preparation and reactions of organocerates.
Organomercurials: Preparation. Electrophilic substitution reactions. Solvomercuration-de-mercuration and cyclopropanation of alkenes. **4h**

Heterocyclic Chemistry-I
Small ring heterocycles: Properties and reactions of 3- and 4- membered heterocycles:- oxiranes, thiranes, aziridines, azetidines, oxetanes and thietanes. **4h**
Benzo-fused heterocycles: Synthesis and reactions of benzofurans, benzothiophenes, benzoxazoles, benzothiazoles and benzimidazoles. **3h**
Six-membered heterocycles with two or more heteroatoms: Synthesis of Diazines, triazines, tetrazines and thiazines. **2h**

UNIT-IV

Heterocyclic Chemistry-II
Seven and large membered heterocycles: Synthesis and reactions of azepanes, oxepines, thiepines, diazepines, thiazepines, azocines, diazocines, dioxocines and dithiocines. **4h**
Heterocycles containing P, As, Sb and Bi: Synthesis of 5- and 6- membered heterocycles with P, As, Sb and Bi. **3h**
Mesoionic compounds: General classification, chemistry of some important meso-ionic heterocycles of type-A and type-B and their applications.. **6h**

SUGGESTED BOOKS

1. Organometallic Chemistry, R. C. Mehrotra and A. Singh, Wiley Eastern, 1991.
2. The Organometallic Chemistry of the transition metals, R. H. Crabtree, 1988.
3. Principles and application of the organotrnsition metal chemistry, J. P. Collman, L. S. Hegedus, University Science books, 1980.
4. An introduction to Organometallic Chemistry, A. W. Parkins and R. C. Poller, Macmillan, 1986.
5. Modern Synthetic Reactions, H. O. House, W.A. Benjamin, California, 2nd Edn. 1972.

6. Organometallics, Vol. 1 & 2, M. Bochmann, Oxford Chemistry primers, Oxford University Press, 1994.
7. Advanced Organic Chemistry, J. March, 4th Edn. John Wiley, 2008.
8. Organotransition metal chemistry, S. G. Davies, Pergamon Press, Oxford, 1982.
9. Heterocyclic Chemistry, Vols. 1-3, R. R. Gupta, M. Kumar and V. Gupta, Springer Verlag.
10. The Chemistry of Heterocycles, T. Eicher and S Hauptimann, Thieme.
11. Heterocyclic Chemistry, J. A. Joule, K. Mills and G. F. Smith, Chapman and Hill.
12. Heterocyclic Chemistry, T. L. Gilchrist, Longman Scientific Tech.
13. Contemporary Heterocyclic Chemistry, G. R. Newkome, and W. W. Paudler, Wiley-Inter Science.
14. An introduction to Heterocyclic Compounds, R. M. Acheson, John Wiley.
15. Comprehensive Heterocyclic Chemistry, A. R. Katritzky and C. W. Rees, Eds. Pergamon Press.
16. Stereochemistry of Organic Compounds, D Nasipuri, New-Age International, (1999).

C-402 OC STEREOCHEMISTRY AND RETROSYNTHETIC ANALYSIS

52 Hours

STEREOCHEMISTRY

UNIT-I

Optical activity in the absence of chiral atoms **5h**

Chirality in biphenyls, adamentanes, ansa compounds, cyclophanes, *trans*-cyclooctene, catenanes, rotaxanes and helicenes. Assignment of R, S- configuration to these classes of compounds.

Optical activity due to the presence hetero atoms **4h**

Chirality of organic compounds due to the presence of silicon, nitrogen, phosphorous, arsenic and sulphur atoms. Determination of R,S-configuration of these compounds using CIP rules.

Transannular reactions **3h**

Conformational analysis of medium rings.

Trasnannular reactions: Hydrolysis of medium ring epoxides and bromination of C_8–C_{10} cyclic dienes.

UNIT-II

Determining absolute and relative configuration **10h**

i). Chemical correlation of configuration: Methods without involving the chiral centre. Chemical transformation involving the chiral centre. Chemical correlation involving diastereomers.

ii). Methods based on comparison of optical rotation: Distance rule, Rule of shift, Rule of optical superposition, Mill's rule, Method based on molecular rotation difference

iii) The method of quasi-racemate.

iv). Use optical rotatory dispersion curves: α-axial haloketone rule and its applications, octant rule (application of these rules in the determination of absolute configuration of substituted cyclohexanones, decalones and cholestanones).

v). Method based on anomalous X- ray scattering.

RETROSYNTHETIC ANALYSIS

Disconnection approach **6h**

Introduction to synthons, and synthetic equivalents, disconnection approach. Basic principles and terminologies used in disconnection approach. One group C-X and two group C-X disconnections. Chemoselectivity, reversal of polarity, cyclisation reactions.

UNIT-III

Protecting groups **4h**

Principle of protection of alcohols, amines, acids and carbonyl groups

C-C one group and C-C two group disconnections **10h**

Synthesis of alcohols, carbonyl compounds and alkenes. Use of acetylides and aliphatic nitro compounds in organic syntesis. Diels-Alder reaction, 1,3-difunctionalised compounds, α,β-

unsaturated compounds, carbonyl compounds condensations, 1,5- difunctionalised compounds. Micheal addition and Robinson annelation.

UNIT-IV

Ring Synthesis **4h**

Synthesis of saturated heterocycles and 3-, 4-, 5- and 6-membered rings.

Synthesis of some complex molecules using disconnection appoach **6h**

Aromadendrene, longifloene, cortisone, reserpine, vitamin-D, juvabione, fredericamycin-A and Lycorane.

SUGGESTED BOOKS

1. Stereochemistry of carbon compounds, E. L. Eliel, S. H. Wilen and L. N. Mander, John Wiley & Sons, 1994.
2. Stereochemistry, Potapov, MIR, Moscow, 1984.
3. Stereochemistry, Nasipuri, D, New Age, 1999.
4. Advanced organic chemistry, J. March, 4th Edn. John Wiley, 2008.
5. Organic Chemistry, R. E. Ireland Prentice-Hall India, New Delhi, 1975.
6. Some modern methods of Organic Synthesis, W. Caruthers, Cambridge Uni. Press London, 2nd Edn., 1998.
7. Stereochemistry of organic compounds- Principle and applications, D. Nasipuri, 2nd Edn., New Age International Publishers, 2001.
8. Organic synthesis: The synthon approach, S. Warren, John Wiley & Sons, New York, 1st. Edn. 1983.
9. Designing organic synthesis: A disconnection approach, S. Warren, John Wiley & Sons, New York, 2nd Edn. 1987.
10. Organic synthesis, C. Willis and M. Wills, Oxford University Press, 1995.
11. Organic synthesis: Concepts, methods and starting materials, J. Furhfop and G. Penzillin, Verlag VCH.
12. Principles of organic synthesis, R. Norman and J. M. Coxon, Blackie Academic & Professional.
13. Advanced organic chemistry Part B, F. A. Carrey and J. Sundberg, Plenum Press, 1999.
14. Organic chemistry Vol. 2, 6th Edn., I. L. Finar, Longman, 1992.

C-403 OC ORGANIC SYNTHESIS

52 Hours

UNIT-I

C-C and C-N bond forming reactions **12h**

Darzen's reaction, Use of acetylides in C-C bond formation reactions. Acid-catalyzed self condensation of olefins, Prins reaction, Shapiro reaction, Dieckmann cyclization, Robinson annulations, Hofmann-Loeffler-Freytag reaction. Hofmann-Martius reaction. Acyloin condensation. Houben-Hoesch reaction.

Stork-enamine synthesis. Meyer synthesis. Use of nucleophilic nitrogen and electrophilic carbon (NH_3, amines and nitrite as nucleophiles in substitution, NH_3 and amines in addition to ketones and aldehydes) and electrophilic nitrogen and nucleophilic carbon (nitration, nitrosation) for the bond formation reactions (including Chichibabin reaction, Skraup synthesis, Mitsunobu reaction, N-Nitroaromatic amine rearrangement, Fisher-Hepp reaction. Japp- Klingemann reaction).

UNIT-II

Reagents in organic synthesis **7h**

Use of the following in organic synthesis and functional group tansformations**.**

Aluminium *iso*-propoxide, NBS, LDA, DCC, DDQ, Corey-Chaykovsky reagent, Raney-Nickel, diazomethane, TMS-chloride, 1,3-Dithiane (reactivity and umpolung), PPA, Yamaguchi reagent. Woodward and Prevost hydroxylation.

Oxidations-I **5h**

Cr (VI) oxidants, Mn (VII) oxidants, OsO_4, SeO_2, Pb $(OAc)_4$, HIO_4, Ag_2O, DMSO.

UNIT-III

Oxidations-II **4h**

ozone, peroxides (H_2O_2, *t*-BuOOH, dibenzoylperoxide) and peracids (Preparation, properties and applications of CF_3COOOH, *m*-CPBA, momoperphthalic acid) as oxidizing agents. Dess-Martin oxidation.

Reductions **9h**

Complex metal hydrides, dissolving metal reductions (including Birch, Benkeser, Clemmensen reductions), diimide reduction, catalytic hydrogenation (homogeneous and heterogeneous), organoboranes as reducing agents. Wolf-Kishner reduction, McMurry reaction. Pummer, Willgerdot, Corey-Bakshi-Shibata and Tishchenko reactions.

UNIT-IV

Asymmetric Synthesis **15h**

'*ee'* and methods of determination of '*ee'*.

Stereoselectivity: classification, terminology and principle.

Asymmetric synthesis and asymmetric induction.

Double diastereoselection and double asymmetric induction.

Acyclic stereoselection: Addition of nucleophiles to carbonyl compounds (1,2- 1,3- and 1,4-asymmetric induction). Asymmetric aldol condensation. Addition of allylmetal and allylboranes to carbonyl group.

Diastereoselection in cyclic systems: Nucleophilic addition to cyclic ketones (formation of axial and equatorial alcohols, catalytic hydrogenation, alkylation, diastereoselective oxidations and stereoselective cyclization of poylenes).
Enantioselective synthesis: Reduction with chiral hydride donors [(S)-PBMgCl, (-)-^{i}BOAlCl$_2$, alpine-borane, (S)-BINAL-H, (R,R)-DIOP, and (S,S)-CHIRAPHOS). Enantioselective alkylation of ketones *via* hydrazones. Enantioselective alkylation with chiral PTC. Enantioselective Michael addition. Enantioselective intramolecular aldol condensation. Use of (+)- and (–)- DET in asymmetric epoxidation.
Polymer-bound chiral catalysts in asymmetric induction.
Asymmetric amplification.

SUGGESTED BOOKS

1. Advanced organic chemistry, J. March, 4th Edn. John Wiley, 2008.
   Organic synthesis, R.E.Ireland, Prentice-hall India, New Delhi, 1975.
2. Understanding organic reaction mechanisms, A. Jacob, Cambridge Univ Press, 1997.
3. Introduction to organic chemistry, A. Streitweiser, Jr and C. H. Heathcock, Macmillan, 1985.
4. Physical and mechanistic organic chemistry, R. A.Y. Jones, 1st Edn. Cambridge Univ Press, 1979.
5. Modern synthetic reactions, H. O. House, W. A. Benjamin, California, 2nd Edn. 1972.
6. Some modern methods of organic synthesis, W. Carruthurs, Cambridge Univ. Press, London, 2nd Edn. 1978.
7. Mechanisms of molecular migration, Vols I & II, B.S. Thyagarajan, Pergamon Press, Oxford, 1979.
8. Comprehensive organic chemistry, D. Barton and W. D. Wallis, Pergamon Press, Oxford, 1983.
9. Organic chemistry Vol. II, I. L. Finar 6th Edn. Longman, 1992.
10. Organic reaction Mechanisms, 3rd Edn., V. K. Ahluwalia and R. K. Prashar, Narosa, New Delhi, 2005.

C-404 OC MEDICINAL ORGANIC CHEMISTRY

52 Hours

UNIT-I

Pharmacokinetics, Pharmacodynamics, Theories of drug activity& Drug design

Basics of drug receptor interactions. Theories of drug activity. Hansch equation. Computer-aided drug design and molecular modeling. **4h**

Steroids

Occurrence. Nomenclature, basic skeleton, Diels hydrocarbon and stereochemistry. Isolation, structure and structural elucidation of sterols and bile acids (determination of ring size, nature of side chain, position of angular methyl and stereochemistry of ring junctions). Sex hormones and corticosteroids. Synthesis of cholesterol, estrone, progesterone, androsterone, testosterone. Photo products of ergosterol- vitamins D. Barton reaction for the synthesis of aldosterone.

Marker degradation. Brief discussion of homosteroids, norsteroids and oral contraceptives. Synthesis of (*dl*)-norgestrel and ethinyl oestradiol. **13h**

UNIT-II

Antibiotics

Structure elucidation and synthesis of streptomycin, penicillins, cephalosporin-C, chloromycetin and tetracyclins (terramycin and aureomycin). **10h**

UNIT-III

Mechanism of drug action and synthesis of the following classes of drugs, with recent developments:

Antipyretics, analgesics and non steroidal anti-inflammatory drugs: Aspirin, paracetamol, phenacetin, novalgin, phenylbutazone and ibuprofen.

Antidiabetics: Sequence of A- & B- chains of insulin, glibenclamide, metformin, ciglitazone.

Antihistamines: Methapyrilene, chlorpheniramine.

Antivirals **:** Acyclovir, amantidine, rimantidine and zidovudine.

Antineoplastic agents: Introduction, cancer chemotherapy, special problems, role of alkylating agents and antimetabolites in treatment of cancer. Mention of carcinolytic antibiotics and mitotic inhibitors. Synthesis of mechlorethamine, cyclophosphamide, melaphan, uracil mustards and 6-mercaptopurine. Recent development in cancer chemotherapy. Hormone and natural products.

Cardiovascular drugs: Introduction, cardiovascular diseases, drug inhibitors of peripheral sympathetic function, central intervention of cardiovascular output. Direct acting arteriolar dilators. Synthesis of amyl nitrite, sorbitrate, diltiazem, quinidine, verapamil, methyldopa, atenolol, oxyprenol.

13h

UNIT-IV

Local anti-infective agents:

Introduction and general mode of action. Synthesis of sulphonamides, furazolidone, nalidixic acid, ciprofloxacin, dapsone, aminosalicyclic acid, isoniazide, ethionamide, ethambutal, fluconazole, econozole, griseofulvin, chloroquin and primaquin.

Psychoactive drugs- chemotherapy of the mind:

Introduction, neurotransmitters, CNS depressants, general anaesthetics, mode of action of hypnotics, sedatives, anti-anxiety drugs, benzodiazepines, buspirone, neurochemistry of mental diseases. Antipsychotic drugs- the neuroleptics, antidepressants, butyrophenones, serendipity and drug development, stereochemical aspects of psychotropic drugs. Synthesis of chlorpromazine, diazepam, oxazepam, chlorazepam, alprazolam, phenytoin, ethosuximide, trimethadione, barbiturates, thiopental sodium, glutethimide. **12h**

SUGGESTED BOOKS

1. Burger's Medicinal Chemistry and Drug Discovery, Vols. 1-6 Ed. D.J. Abraham, John Wiley, 2003
2. Foye's Principles of Medicinal Chemistry, 6th Edn., T L Lemke and D A Williams Eds., Lippincott, Williams and Wilkins, 2007
3. An Introduction to Medicinal Chemistry, P Graham, III Ed., Oxford, 2006
4. Medicinal Chemistry, N Weaver, Oxford, 2006
5. Goodman and Gilman's Pharmacological Basis of Therapeutics, 11th Edn., Tata McGraw-Hill, 2005.
6. The Organic Chemistry of Drug Design and Drug Action, R B Silverman,II Edn, Academic Press, Amsterdam, 2004.
7. Wilson and Gisvold's Text Book of Organic Medicinal and Pharmaceutical chemistry, J H Block and J M Beale, Jr., Eds., Lippincott, Williams and Wilkins, 2003.
8. Medicinal Chemistry – G R Chatwal, Himalaya, New Delhi, 2002
9. Instant Notes Medicinal Chemistry, P Graham, Viva, New Delhi, 2002
10. Medicinal Chemistry, A Kar, Wiley, 2000.
11. An Introduction to Drug Design, S.S. Pandey and J.R. Dimmock, New Age International, 1999.
12. Strategies for Organic Drug Synthesis and Design, D. Lednicer, John Wiley,1998.
13. Synthetic drugs, G. R. Chatwal, Himalaya, New Delhi, 1995.
14. Natural Products Chemistry Vol 1 and 2, G R Chatwal, Himalaya, New Delhi, 1990
15. Comprehensive Organic Chemistry, Vol. 5 (Antibiotics), D. H. R. Barton, W. D. Ollis, Pergamon Press, NY, 1979.
16. Organic chemistry Vol.II, I. L. Finar, 6th Edn. Longman, 1992.
17. Total synthesis of natural products: The chiral approach Vol.III, S. Hanessian Pergamon Press, 1983.
18. Total synthesis of steroids, Akhaun & Titov, Jerusalem, 1969.
19. Medicinal natural products: A biosynthetic approach, P. M. Dewick. John Wiley, Chichester, 1997.
20. Natural products: Their chemistry and biological significance-J. Mann, R. S. Davidson, J. B. Hobbs, D. V. Banthorpe & J. B. Harborne, Longman, UK, 1994.
21. Natural products chemistry Vol. I & II, K. Nakanishi, T. Goso, S. Ito, S. Natori & S. Nozoe, Academic Press, NY, 1974.
22. Chemistry of natural products Vol. I & II, O. P. Aggarwal, Goel Publishing House, 6th Edn. 1982.
23. Total synthesis of natural products: The chiral approach Vol.III, S. Hanessian Pergamon Press, 1983.
24. Interpretation of the UV spectra of natural products, A.I. Scott, Pergamon Press, Oxford, 1964.

ORGANIC CHEMISTRY PRACTICALS
(2 days a week, 4 hours a day)

C-405 ORGANIC CHEMISTRY PRACTICALS - V

I – PREPARATIONS

1. Preparation of NBS from succinic acid and its application in allylic bromination reactions.
2. Preparation of benzpinacolone from benzophenone.
3. Generation of benzyne and its trapping with tetracyclone.
4. Preparation of 2-phenylindole from phenylhydrazine
5. Anthrone from Anthracene.
6. Synthesis of stilbene.
7. Synthesis of benzocaine from 4-nitrobenzoic acid.
8. Preparation of tetraphenyldihydrophthalic anhydride from N-phenylglycine.
9. Preparation of 2,4,5-triphenyloxazole from benzoin
10. Biosynthesis of ethanol from sucrose.
11. Synthesis of Methyl Red
12. Synthesis of 1-bromo-2-naphthol from 2-naphthol
13. Synthesis of Hippuric acid
14. 1,2,3,4- Tetrahydrocarbazole
15. Diels-Alder reaction of anthracene with maleic anhydride
16. Synthesis of 2,3-diphenylquinoxaline

II-INSTRUMENTAL METHODS IN ORGANIC ANALYSIS

1. Recording/predicting/downloading from web sites the UV, IR, NMR and GC-MS/mass spectra of the compounds prepared in C-105/205/305 (Organic Practical – I), C-106/206/306 (Organic Practical – II), C-405 (Organic Practical – III) and C- 406 (Organic Practical – IV).

2. Structural elucidation of organic compounds with the help of spectra provided by the instructors/examiners.

C-406 ORGANIC CHEMISTRY PRACTICALS - VI

I - QUALITATIVE ANALYSIS

Separation of a binary mixture of organic compounds and identification of the separated components by systematic qualitative organic analysis.

II – QUANTITATIVE ANALYSIS

Estimations:

1. Estimation of Nitro group by reduction using $SnCl_2$.
2. Estimation of Nitrogen by Kjeldahl's method.
3. Estimation of an acid in presence of an amide.
4. Estimation of an ester in the presence of an acid.

SUGGESTED BOOKS

1. Semi-micro qualitative organic analysis, Cheronis, Entrikin & Hoanett.
2. Preparation of organic intermediates, D. A. Hirley, John Wiley.
3. Text book of practical organic chemistry, A. I. Vogel, Pearson, 5th Edition, Delhi, 2004.
4. A laboratory manual of qualitative organic analysis, H.T. Openshaw, Univ. Press, 1999.
5. Organic Synthesis collective Vols. I to X, 1956-1999.
6. Natural products, Laboratory manual, Ikan, 2000.
7. Organic experiments, L. F. Fieser, 2nd Edn. D. C. Heath & Co. USA, 1974-2000.
8. Practical organic chemistry F.G. Mann and B. C. Saunders 4th Edn. Longman, 2002.
9. Comprehensive practical organic chemistry : Preparation and quantitative Analysis, V. K. Ahluwalia, R. Aggarwal, Universities Press (India), 2000.
10. Comprehensive practical organic chemistry: Qualitative analysis, V. K. Ahluwalia, S. Dhingra, Universities Press (India), 2000.
11. An advanced course in practical chemistry, A. Ghoshal, B. Mahapatra and A. K. Nad, New central book agency, Calcutta, 2000.
12. Advanced practical organic chemistry, J. Mohan, Vol. I and II, Himalaya Publishing House, 1992.
13. Practical organic chemistry (Quantitative analysis), B. B. Dey, M V Sitaraman and T. R. Govindachari, Allied Publishers, New Delhi, 1992.
14. Laboratory Techniques in Organic Chemistry, V K Ahluwalia, Pooja Bhagat and Renu Aggarwal, I K international Publishing House, New Delhi, 2005.
15. Intermediates for Organic Synthesis, V K Ahluwalia, Pooja Bhagat, Ramesh Chandra and Renu Aggarwal, I K international Publishing House, New Delhi, 2005.

ORGANIC CHEMISTRY

C-407: PROJECT WORK
(8 Hours PER WEEK)

FOURTH SEMESTER

PHYSICAL CHEMISTRY SPECIALISATION

C-401 PC APPLIED ELECTROCHEMISTRY 52 Hours

UNIT-I

13h

Electroanalytical methods

A. Voltametry: Definition, concentration polarization, ideal and non-ideal polarized electrodes, Faradaic and non-faradaic currents.

Polarography- Construction of dropping mercury electrode (DME), advantages and limitations.Principle of normal dc polarography, half-wave potential, qualitative analysis using polarograms.Types of currents obtained at a DME. Ilkovic equation, factors affecting diffusion controlled current, quantitative analysis based on Ilkovik equation. current-potential relationfor a cathodic wave, anodic wave and composite wave,test for the reversibility of a process at DME, factors that set the sensitivity and selectivity limits in normal dc polarography.

*Advanced polarographic techniques:*Tast polarography, normal pulse polarography, differential pulse polarography, ac polarography.

Stripping voltametry: Hanging drop mercury electrode (HDME), principles and applications of cathodic and anodic stripping voltammetry.

*Cyclic voltammetry:*Principle, experimental setup,qantitative analysis.Diagnostic criteria for reversible, quasi-reversible and irreversible processes.Study of coupled chemical reactions like E_rC_r, C_rE_r and $E_rC_iE_r$.

B. Chronomethods: Basic concepts, methodology and applications of chronoamperometry, chronopotentiometry and chronocoulometry.

C. Hydrodynamic electrodes: Construction and use of rotating disc and rotating ring disc electrodes in the electrochemical studies.

D. Membrane electrodes: Ion-selective membrane electrodes-construction and applications of solid state and liquid membrane electrodes, ion selective field effect transistor and Molecular(gas) sensing probes.

E. Problems solving.

UNIT-II

13h

Electrochemical energy conversion and storage.

*Batteries:*History and basics, classification, characteristics with units-voltage, current,capacity, electricity storage density, energy density, power density, energy efficiency, cycle life, shelf life.

Primary batteries: Construction, reactions and uses of Leclanche' dry cell, alkaline Leclanche cell, zinc-silveroxide cell.

Secondary batteries: Construction, working (charge-discharge reactions), applications advantages and of Pb-acid and Ni-Cd batteries.

Hybrid Batteries: Metal-air batteries- meaning, Zn-air battery, Fe-air battery, Charging of metal-air battery, Metaloxide-hydrogen/hydride batteries, advantages and limitations of these cells

Lithium batteries: Primary and secondary lithium battery,Li-ion battery and Lithium ion-polymer battery.

*Electrochemical supercapacitors:*comparative meaning of capacitor, electrolytic (super) capacitor and ultracapacitors, materials for construction, applications, advantages and limitations.

Fuel cells: Energy efficiency of electrochemical and thermal conversion (Carnot limitation).Definition of fuel cell, classification.Fuel cell efficiency- thermodynamic, electrochemical, practical efficiency.Electrode (anode and cathode) mechanism of fuel cell, Brief description on construction, working principle and applications of each type fuel cells. An account of electrocatalysts, proton exchange membrane (PEM) fuel cells anddirect methanol fuel cell. Problems solving.

UNIT-III

13h

Surface Modification techniques (Metal finishing)

Definition, important processes of metal finishing, technological importance of metal finishing.

*Electroplating:*Definition, theory and mechanism of electroplating, effect of plating variables on the properties of electrodeposits, comparative account of complexing and non complexing baths(general treatment), additives in the plating bath and their significance.

Metallic coating: Preparation of substrate surface, electroplating of Cu and Cr. Applications of Au and Ag platings.

Solar selective coatings: Characteristics, methods of preparation and applications.

Techniques of electroplating: Galvanizing, Anodizing, Phosphating, Chromating.

Electroless plating: Definition, advantages over electroplating, pretreatment of substrates, an account of electroless plating of Ni including applications.

Testing of coats: Principles of measurement of coating thickness, adhesion, porosity, corrosion resistance, reflectance, and hardness.A brief account of surface analysis by XPS and AES techniques.

Indusrtial effluent treatment: An account of removal of toxicants like, CN, Cr, Pband Cdfrom plating industrial effluent. Problems solving

Electrochemical synthesis

Special features of electrochemical synthesis compared to conventional synthesis-reaction variables (electrode material, electrode potential, solvent, supporting electrolyte, temperature, agitation) in electrochemical synthesis. Two examples for electrorganic, electroinorganic and electrochemical nanoparticles synthesis with mechanism.

UNIT-IV

13h

Corrosion and its Prevention

Introduction, dry and wet corrosion, theories and mechanisms of wet (electrochemical) corrosion, thermodynamic aspects of corrosion, kinetic aspects- determination of rates of corrosion by linear polarization, Tafel extrapolation and impedance techniques.Factors influencing the rate of corrosion- metal and environmental.

Methods of corrosion prevention: Cathodic protection, anodic protection, use of corrosion inhibitors, use of organic coatings.

Passivity: Definition, corrent potential diagram, characteristics of passivity, theory and mechanism of passivation, flade potential, trans passivity. Use of ellipsometric technique in the study of passivating films. Problems solving

Bioelectrochemistry

The electrochemical interface between biomolecules, cellular membrane, transmembrane potential, bilayer lipid membranes, electroporation, biological electron transport, electrochemistry of redox enzymes, biological membrane and membrane mimics. Biosensors-NADP, glucose, phenolic. Bioelectroanalysis: Electrolysis and Electrodialysis.

SUGGESTED BOOKS

1. Modern Electrochemistry, Vol.1,2A and 2B by Bockris and Reddy, Plenum, N.Y (2000).
2. Polarography and Allied Techniques by V SuryanarayanaRao, Universities Press (india) Pvt. Ltd., Hyderadad (2002).
3. Basic concepts of Analytical Chemistryby S M Khopkar, New Age Internatonal Publishers, third edition, New Delhi, 2008.
4. Electrochemical Methods- Fundamentals and Applications, 2nd Edn, by A J Bard and L R Faulkner, John Wiley & Sons Inc., New York (2001).
5. Chemical and Electrochemical Energy systems by Narayan and Viswanathan, Hyderabad, Universities Press (india) Pvt. Ltd., Hyderadad (2002).
6. Understanding Batteries, RM Dell and DAJ Rand, 2001.6. Fuel cells and their applications, Karl kordesh, gunter,Simader, VCH-Weinheim, Cambridge,1996.
7. Fundamentals of electrochemical deposition, Milan Paunovic and Mordechay Schlesinger, Wiley- interscience publications, New York, 1998
8. Electrodeposition and Corrosion Control, J. M. West, J. Wiley W. Revie (ed.): Corrosion Handbook, Electrochemical Society Series, John Wiley and Sons (2000).
9. Electrochemistry and corrosion science, Nestor Perez, Springer (india) pvt. Ltd., 2004
10. Principles and Prevention of Corrosion, D. A. Jones, Macmillan Publ. Co. (1996).
11. Bioelectrochemistry: Fundamentals, experimental techniques and application, P. N. Bartlett, Wiley& Sons (2008).
12. Synthetic organic Electrochemistry by A M Fry, 2nd Edn, Wiley 1989 .

C-402 PC CHEMISTRY OF MACROMOLECULES AND ADVANCED PHOTOCHEMISTRY

52 Hours

UNIT-I

13h

Molecular weight determinations:

Determination of molecular weight average by (i) osmotic pressure, Donnan membrane equilibrium**,** (ii) Light scattering, fundamental concepts, scattering from number of particles, Rayleigh scattering from solutions of macromolecules, scattering by macromolecules, (iii) Sedimentation velocity, (iv) Sedimentation equilibrium (v) density gradient sedimentation (vi) viscosity: specific viscosity, relative viscosity, intrinsic viscosity, Determination of molecular weight and size of macromolecules (vii) electrophoresis: isoelectric point, isoelectric focusing techniques and determination of molecular weight by electrophoresis technique.

Derivation of relevant expression in each above experimental cases and use of these above methods in evaluation of shapes and confirmations of macromolecules

UNIT-II

13h

Thermodynamics of Polymer solution:

Partial molar and partial specific quantities, Chemical potential of macromolecular solution Gibbs-Duhem equation, concepts of second viral coefficient and excluded volume. Mathematical expressions for various models postulated for the shapes of macromolecules in solution; spheres, ellipsoid, long rod and flexible random coil

Spectroscopic studies of Macromolecules:

Determination of structure of macromolecules: Spin forbidden transitions, symmetry forbidden transitions,

NMR: Introduction, resonance condition for a nuclear spin in the presence of an external magnetic field (quantum mechanical and classical description), nuclei suitable for NMR study, effect of electron shielding on nuclear magnetic resonance condition, spin- spin interaction,

ESR: Introduction, resonance condition for an electron, relation between an absorption line and its derivative

UNIT-III

13h

IR: Introduction to microwave spectroscopy, some typical infrared absorption bands found in biological systems, infrared dichroism, simple numerical problems for the calculation of moment of inertia and force constant.

Electronic spectroscopy: Introduction, selection rules, allowed and forbidden transitions, some common chromophores and their approximate maximum absorption wavelengths, relationship of wavelength to color, hypochromism, UV-visible dichroism, effect of increased conjugation, charge transfer interaction, effect of pH on the UV-visible spectrum.

ORD and CD: Introduction, plane polarized and circularly polarized radiations, molecular symmetry and optical activity, polarized light and optical rotation, circular dichroism, Cotton effect and optical rotatary dispersion (both negative and positive ORD and Cotton effect), Drude's equation

Advanced Photochemistry-I

Born-Oppenheimer approximation, identification of molecular orbitals based on symmetry properties and symmetry elements, spectroscopic term symbols for molecules, direct product rule for assigning molecular symmetry from orbital symmetry, potential energy diagram for molecular oxygen electronic energy states in relation with the absorption spectrum, notation for excited states of organic molecules.

UNIT-IV

Advanced Photochemistry-II **13h**

Excited state dipole moment, excited state acidity constant pk* values (Forster's cycles), excited state redox potential, flash photolysis, Wigner's spin conservation rule.

Photophysical process: Jablonski diagram, quenching and collisional deactivation, Stern-Volmer Plot, Fluorescence: General principle, energy level diagram, mirror image relationship, Kasha's rule, spectro fluorimetry, sensitized delayed fluorescence. Phosphorescenc, Spectro phosphorimetry, lasers, chemiluminscence, excimers and exciplexes.

Organic and inorganic photochemistry

Reaction in compounds containing cabonly groups, photoreduction and related reactions photocyclo addition reactions, bonding and anti bonding molecular orbitals of ethylene 1,3 butadiene and allyl systems, orbital symmetry and chemical reaction, elctrocyclic reactions, Woodward and Hoffmann correlation rules applied to 1,3 butadiene and 1,3, 5-hexatriene, comparison of thermal and photochemical reaction.

Energy levels of inorganic transition metal complexes, redox properties of $[Ru(bpy)_3]^{2+}$, excited state outer sphere electron transfer reactions, inner sphere, mechanism

SUGGESTED BOOKS

1. Fundamentals of photochemistry, K.K. Rohatgi Mukhergee, Wiley Eastern Limited (1986)
2. Photochemistry, Carol E Wayne and Richard P Wayne, Oxford University Press (1996)
3. Introduction to Semiconductor Materials and devices M S Tyagi, John Wiley and sons (1991)
4. Organic Photochemistry, J. M. Cozen and B. Halton, Cambridge University Press (I st Edition) 1974
5.Molecular Reactions and Photochemistry, C H Deputy and D S Chapman, Prentice Hall India, New Delhi (1st Edition) , 1972.
6. Concepts of Inorganic photochemistry, A. W. Adamson and P D Fleischaves Wiley.
7. Elements of Inorganic Photochemistry G. J. Ferranti,Wiley.
8. Physical Chemistry, P. W. Atkins, Julio de Paulo ELBS 7th Edition (2002)
9. Text book of polymer science F. W. Bilmeyer (John Wiley) London 1994
10 Ploymer science V. R. Gowariker, N, V. Viswanathan & T. Sreedhar (Wiley edition) New Delhi 1990
11.Introduction to physical polymer science L. H. Speriling Wiley Interface New York (1986)
12. Principles of polymer chemistry P J Flory Cirnell University Press Ithaca (1953)
13 Principles of polymerization G. Odian 3rd edition Wiley inter science New York 1992
14. Polymer sscience and technology J. R. Fried (Prentice Hall), New Delhi

C-403 PC REACTION KINETICS AND MECHANISMS

52 h

UNIT-I

Reactions in solution

Cage effect, Reaction between gas phase and solution phase. Influence of solvent on reaction rate (Double sphere model), Primary and secondary isotope effects on reaction rates, Linear free energy relationships (LFER): Thermodynamic implications of LFER, Inductive and electromeric effects on reaction rates, Effect of substituents on activation energies, Hammett and Taft equations, Swain-Scott and Edward equations, Winstein Grunwald relationship, Isokinetic relationship- Evaluation of Isokinetic temperature and its significance, Diffusion and activation controlled reactions. Microscopic reversibility. Volume of activation-entropy of activation, Significance of volume of activation. **13 h**

UNIT-II

Reaction mechanisms

General approaches and importance of reaction mechanism. Kinetics and mechanisms of: Decomposition of N_2O_5, Halogenation of acetone, Dehydrogenation of ethane, Hypohalite-iodide reaction, Pyrolysis of butane and Nucleophilic and electrophilic substitution reactions. Mechanisms of N-haloamines. **6h**

Chain and Complex reactions

Introduction, Methods of production and identification of free radicals, Kinetics of branched chain reactions, explosion limits of H_2-O_2 reaction. Oscillatory reactions – Introduction, Oxidation of malic acid by bromate ion catalysed by Ce(III), Kinetics and mechanisms of polymerization reactions: Addition (Free radical, Anionic and Cationic) and Condensation polymerization. **7h**

UNIT-III

Kinetics of catalyzed reactions

Heterogeneous catalysis- Intermediate compound formation theory and adsorption theory. Activation energies for catalysed reactions. Role of surfaces in heterogeneous catalysis, Acidity functions-Relationship between the rate constant and acidity function; Hammett-Zucker hypothesis, Bunnett plot. N-Haloamines-classification and reactive species. Ru(III) chloride catalysed oxidation reactions of some alcohols and aminoacids by chloramine-T in acid and alkaline media, Deduction of reaction mechanisms, rate laws, catalytic coefficients, equilibrium and decomposition constants. Industrial catalysts – catalyst carrier, catalyst promoter, catalyst inhibitor and catalyst poison. Role of surfaces in heterogeneous catalysis. **13h**

UNIT-IV

Pharmacokinetics

Basic considerations, Objectives, Kinetic orders of reactions, Plasma drug concentration- time profile, Pharmacokinetic and pharmacodynamic parameters, Protein binding of drugs, Factors affecting protein-drug binding, kinetics of protein-drug binding, Drug dissolution rate. Bioavailability- objectives and enhancement of bioavailability, Physico-chemical factors

affecting bio-availability. Compartment modeling: Introduction, one compartment open model, Calculation of elimination rate constants. **7h**

Molecular reaction dynamics

Reactions in molecular beams, Potential energy surface for H + H_2 reaction, Theoretical calculation of activation energies of potential energy surfaces, Transmission co-efficient, Quantum mechanical tunneling, Reaction co-ordinate, Symmetry numbers and Statistical factors, Mean free path, Reaction rates and cross sections. **6h**

SUGGGESTED BOOKS

1. Chemical Kinetics, K. J. Laidler 3rd Edition (Mc-Graw Hill Inc.) New York, (2007).
2. Kinetics and Mechanism, Frost and R.G. Pearson (John-Wiley) New Yoork, (1962).
3. Physical Chemistry, P. W. Atkins 7th Edn, (Oxford) (2004).
4. Introduction to Molecular Dynamics and Chemical Kinetics, G.D. Billing and Milkelson. (Wiley Interscience), (1996).
5. Organic Reaction Mechanism, R. K. Bansal (Mc- Graw Hill) New Delhi, 1978.
6. Reaction Mechanism in Organic Chemistry, S.M. Mukheji, S.P.Singh and R.P. Kapoor (Mc. Millan India Ltd.,) Bangalore, (1978).
7. Catalysis, J. K. Kuriacose (McMillan India Ltd..,) (1991).
8. Text book of Polymer Science, F. W. Billmeyer (John-Wiley) 1984.
9. Introductory polymer Chemistry, G. S. Misra (Wiley Eastern Ltd.,) New Delhi, 1993.
10. Polymer Science, Gowrikar et al (Wiley Eastern Ltd.,) New Delhi, 1990.
11. Introduction to Physical Organic Chemistry, R. D. Gilliom (Additions-Wesley) USA, 1970.
12. Physical Organic Chemistry, Reaction Rates Equilibrium and Mechanisms, L. P. Hammett, 2nd Edn, (Mc-Graw Hill Book. Co.) 1970.
13. Biophysical Chemistry- Priciples and Techniques, A. Upadyayay, K. Upadyayay, N. Nath (Himalaya Publishing House), Mumbai, 1998.
14. Foundation of Chemical Kinetics, S. W. Benson (Mc-Graw Hill), New York, 1960.
15. Comprehensive Chemical Kinetics, Vol-I, Banford and Tipper (Elsevier Publishing Co.,) New York 1969.
16. Physical Chemistry, G. M. Barrow, 5th Edn,, (Tata Mc-Graw Hill), 1992.
17. Principles of Chemical Kinetics, J. E. House (Wm C Brown Publisher) Boston, 1997.
18. Modern Physical Organic Chemistry-V. A. Eric and A.D. Dennis, University Science Books, USA, (2006).
19. Physical Chemistry, R. J. Silbey, R. A. Alberty and M. G. Bawendi; 4th Edn. Wiley (2009)
20. Molecular Reaction Dynamics, Hardy Levin and R. B. Bernstein, Oxford University Press, New York (1974).

C-404 SPECTROSCOPY – III

(Common to Analytical, Inorganic and Physical Chemistry)

52 Hours

UNIT-I

Vibrational spectroscopy **9h**

Vibrational spectra of diatomic, linear and bent triatomic, AB_3, AB_4, AB_5 and AB_6 molecules, spectra of metal complexes: Ammine, amido, Nitro, Nitrito, lattice water, aquo and hydroxo, carbonato, nitrato, sulphato and other acido complexes, cyano and nitrile complexes, cyanato and thiocyanato complexes, mono and multinuclear carbonyl complexes, nitrosyls, phosphines and arsines, ambidentate ligands, ethylenediamine and diketonato complexes

Raman spectroscopy **4h**

Resonance Raman Spectroscopy, Nonlinear Raman effects-Stimulated, hyper and inverse types, Lasers and their use in Raman spectroscopy

Photoacoustic spectroscopy: Basic description and applications **2h**

UNIT-II

Photoelectron spectroscopy **8h**

Basic principles- photoelectric effect, Koopman's theorem, XPS and UPS, spin-orbit coupling in core level spectra, applications of core level spectra-ESCA, chemical shift, Valence level spectra- n, σ and π bands, Auger electron spectroscopy and applications, Electron energy loss spectroscopy- basic principles and applications

Applications to the study of solids

NMR spectroscopy of inorganic molecules **8h**

Proton NMR spectra of metal hydride complexes

NMR spectra of nuclei other than hydrogen: ^{19}F, ^{31}P, ^{11}B NMR spectra of simple compounds, Proton/hydride interactions with ^{103}Rh, ^{183}W, ^{195}Pt and ^{207}Pb in metal complexes/organometallic compounds, Solid State NMR.

UNIT-III

Electron spin resonance spectroscopy **10h**

Basic principles, the position of ESR absorption, significance of 'g' factor, determination of 'g'factor. Electron-nucleus coupling (Hyperfine splitting). ESR spectrometer, electron-electron coupling, double resonance in ESR, ENDOR, ELDOR. Interpretation of ESR spectra and structure elucidation of organic radicals using ESR spectroscopy. Spin density and Mc Connell relationship. Spin polarization for atoms and transition metal ions, spin-orbit coupling and significance of g-tensors, zero/non-zero field splitting, Kramer's degeneracy, application to transition metal complexes (having one to five unpaired electrons) including biological molecules and inorganic free radicals such as PH_4, F_2 and BH_3.

UNIT-IV

Mossbauer spectroscopy **5h**

Basic principles, isomer shift, quadrupole splitting and magnetic hyperfine interactions, application to the study of bonding and structures of Fe^{2+} and Fe^{3+} compounds, Sn^{2+} and Sn^{4+} compounds

NQR spectroscopy **4h**

NQR isotopes, electric field gradients, Nuclear Quadrupole coupling constants, Experimental techniques and applications

X-ray absorption spectroscopy **2h**

Near edge measurements and EXAFS

SUGGESTED BOOKS

1. Physical methods in Inorganic Chemistry, R.S. Drago, Affiliated East West Press Pvt. Ltd., New Delhi (1965).
2. Infrared spectra of Inorganic and Coordination Compounds, K. Nakamoto, Wiley Interscience, New York (1970).
3. Vibrational Spectroscopy: Theory and Applications, D.N. Sathyanarayana, New Age International Publishers, New Delhi (2000).
4. Electronic Absorption Spectroscopy and Related Techniques, D.N. Sathyanarayana, Universities Press, Bangalore (2001).

PHYSICAL CHEMISTRY PRACTICALS
(2 days a week, 4 hours a day)

C-405 PHYSICAL CHEMISTRY PRACTICALS-V

1. Determination of order of the reaction for the hydrolysis of methyl acetate and evaluation of activation parameters
2. Determination of Ea for the hydrolysis of t-butly chloride by conductivity method
3. Kinetics of oxidation of glycine by chloramines-T, determination of order with respect to glycine
4. Study of kinetics of hydrolysis of t-butyl chloride by conductivity method, detmination of rate constant, energy of activation and thermodynamic parameters
5. Degree of hydrolysis of urea-hydrochloride from the study of acid hydrolysis of methyl acetate.
6. Study of acetone-iodine reaction-determination of order with respect to each reactant by ratio variation method.
7. Kinetics of decomposition of H_2O_2- effect of catalyst and promoter.
8. Study of decomposition of diacetone alcohol using dilatometer- Evaluation of catalytic coefficient of OH^- ions, Ea and thermodynamic parameters.
9. Kinetics of oxidation of indigo carmine by chloroamine-T-spectrophotometrically and determination of Ea and thermodynamic parameters.
10. Determination of catalytic efficiency of $RuCl_3$ for the reaction between a primary amine and CAT.
11. Study of the effect of dielectric constant using methanol on the kinetics of the reaction between a primary amine and CAT.
12. Study of effect of salt (ionic strength) on the kinetics of the reaction between potassium persulphate and potassium iodide.
13. Kinetics of autocatalytic reaction between potassium permanganate and oxalic acid.
14. Absorption spectrum of a conjugated dye and verification of quantum mechanics of particle in one dimensional box
15. Spectral interpretation for structure elucidation of simple organic compounds (-COOH, -OH, $-NH_2$, and -Cl) by FT-IR.
16 Powder diffraction pattern of simple salt and determination of lattice type and the parameters.
17. Evaluation of cell parameters from rotational photograph.
18. Demonstration of fluorescence of solution of anthracene in benzene with respective to UV-visible absorption spectra.
19. To construct the phase diagram of a three component systems ($CHCl_3$-acetic acid- water).

C-406 PHYSICAL CHEMISTRY PRACTICALS-VI

1. Study of the complex formation and determination of the stability constant of silver ammonia complex.
2. Determination of the free energy change oa a cell reaction.
3. Determination of mean-ion activity co-efficient of HCl and the study of the effect of ionic strength on the activity co-efficient of Ag^+ ions.
4. Determination of solubility of silver halides in a mixture.
5. Determination of acid and base dissociation constants of an amino acid and hence its isoelectric point by pH metry.
6. Determination of pKa values of a poly basic acid potentiometrically using quinhydrone electrode.
7. Determination of pKa values of a poly basic acid pH metrically.
8. Titration of ferrous ammonium sulphate against potassium dichromate using a bimetallic electrode.
9. Differential potentiometric titrations:
   i) Weak acid against strong base
   ii) Mixture of strong and weak acids against strong base.
10. Conductometric titrations:
    (i) Thorium nitrate with potassium tartrate.
    (ii) Potassium iodide with mercuric perchlorate
    (iii) Acetic acid, monochloro acetic acid and trichloro acetic acid with strong alkali.
11. Determination of hydrolysis constant of aniline hydrochloride conductometrically.
12. Determination of equivalent conductance of a weak electrolyte (acetic acid) at infinite dilution following Kohlarauch law.
13. Spectrophotometric determination of indicator constant (bromophenol blue)
14. Determination of stability constant of a complex formed between salicylic acid and ferric ion by variation of pH.
15. Determination of corrosion rate of:
    (i) Zn in NaOH by weight loss method.
    (ii) Mild steel in HCl by polarization method.
16. Polarography:
    (i). Identification of metal ions in a mixture.
    (ii) Quantitative determination of electroreducible species.
17. Study of the redox behavior of $K_4 Fe(CN)_6/K_3Fe(CN)_6$.
18. Determination of molecular weight of a polymer by viscosity method.

SUGGESTED BOOKS

1. Findlays practical physical chemisty revised by P. B. Levitt, Longman's London (1966).
2. Experiments in Physical Chemistry by Shoemaker and Garland, McGraw Hill International Edn. (1966).
3. Advanced Practical Physical Chemistry by J. B. Yadav, Goel Publications Meerut (1988).
4. Senior Practical Physical Chemistry by B. C. Kosla, Simla Printers New Delhi (1987).
5. Experimental Physical Chemistry by Daniel et al., McGraw Hill, New York (1962).
6. Practical Physical Chemistry by A.M James and P. E. Pritchard, Longman's Group Ltd (1968)
7. Experimental Physical Chemistry by Wilson, Newcombe & others, Pergamon Press, New York (1962).

8. Experimental Physical Chemistry by R. C. Behra and B Behra, Tata McGraw, New Delhi (1983).
9. Experimental Physical Chemistry by V. D. Atavale and Parul Mathur, New Age International, New York (2001)
10. Physical Chemistry Laboratory Principles and Experiments by H. W. Salberg J. I. Morrow, S. R. Cohen and M. E. Green Macmillan publishing Co .new York.
11. Practical's in physical chemistry A. Mordren Approach by P.S Sindhu, Mac. Millan Publishers Delhi (2006).

PHYSICAL CHEMISTRY
C-407: PROJECT WORK
(8 Hours PER WEEK)

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