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BENGALURU CENTRAL UNIVERSITY

SYLLABUS FOR M.Sc CHEMISTRY

**CHOICE BASED CREDIT SYSTEM
(SEMESTER SCHEME)**

2019-2020 onwards

Proceedings of the meeting of the Board of Studies in Chemistry (PG) held on 10th Jan. 2019 in the Department of Chemistry, Central College, Bengaluru Central University, Bengaluru-560 001.

A meeting of the Board of Studies in Chemistry (PG) was held on Thursday the 10th Jan. 2019 at 10.30 am in the Department Library to approve the proposed M.Sc., CBCS syllabus with effective from 2019-2020 onwards.

The BOS, Chairman welcomed the members and as per the agenda the M. Sc., CBCS Chemistry syllabus was placed before the members. The members after careful scrutiny approved the M.Sc., (CBCS) Chemistry syllabus with modifications wherever necessary. The following papers have been thoroughly discussed and the corrections have been incorporated.

I SEMESTER




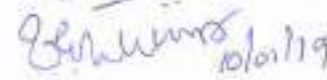



Code No.	Title
Ch-101	Inorganic Chemistry I
Ch-102	Organic Chemistry I
Ch-103	Physical Chemistry I
Ch-104	Analytical Chemistry
Ch-105	Mathematics for Chemists (Soft Core)
Ch-106	Practical-I Inorg/Org/Phy
Ch-107	Practical-II Inorg/Org/Phy
Ch-108	Practical-III Inorg/Org/Phy
Ch-109	Practical-IV Inorg/Org/Phy

II SEMESTER

Code No.	Title
Ch-201	Inorganic Chemistry II
Ch-202	Organic Chemistry II
Ch-203	Physical Chemistry II
Ch-204	Spectroscopy - I
Ch-205	Green Synthesis/Photo Chemistry (Soft Core)
Ch-206	Practical-I Inorg/Org/Phy
Ch-207	Practical-II Inorg/Org/Phy
Ch-208	Practical-III Inorg/Org/Phy
Ch-209	Practical-IV Inorg/Org/Phy

Finally the Chairman thanked all the members.

MEMBERS PRESENT

1	Prof. B. Narayana	-	External member	
2	Prof. Boja Poojary	-	External member	
3	Prof. V. Gayathri	-	Internal member	 10/01/19
4	Prof. S. Hariprasad	-	Internal member	 10-1-2019
5	Prof. P. R. Chetana	-	Internal member	 10/01/19
6	Prof. K. Shivashankar	-	Internal member	 10/1/19
7	Dr. G. Krishnamurthy	-	Internal member	
8	Prof. M. Pandurangappa	-	CHAIRMAN	 10/01/2019

 28/01/2019

Prof. M. PANDURANGAPPA
Coordinator Department of Chemistry
Bengaluru Central University
Central College Campus
Dr. Ambedkar Veedhi,
BENGALURU - 560 001

BENGALURU CENTRAL UNIVERSITY
DEPARTMENT OF CHEMISTRY
CENTRAL COLLEGE CAMPUS
BENGALURU - 560 001
PROPOSED STRUCTURE OF MASTER OF SCIENCE (CHEMISTRY)
(CBCS)

I SEMESTER			II SEMESTER			III SEMESTER			IV SEMESTER		
Code	Name	Credits	Code	Name	Credits	Code	Name	Credits	Code	Name	Credits
Ch-101	Inorganic Chemistry I	4	Ch-201	Inorganic Chemistry 2	4	Ch-301		4	Ch-401		4
Ch-102	Organic Chemistry I	4	Ch-202	Organic Chemistry 2	4	Ch-302		4	Ch-402		4
Ch-103	Physical Chemistry I	4	Ch-203	Physical Chemistry 2	4	Ch-303		4	Ch-403		4
Ch-104	Analytical Chemistry	4	Ch-204	Spectroscopy I	4	Ch-304		4	Ch-404		4
Ch-105	Mathematics for Chemists	2	Ch-205	Green Synthesis/ Photochemistry	2						
Ch-106	Inorganic/Organic/Physical Lab 1	2	Ch-206	Inorganic/Organic/ Physical Lab 1	2	Ch-305	Lab 1	2	Ch-405	Lab 1	2
Ch-107	Inorganic/Organic/Physical Lab 2	2	Ch-207	Inorganic/Organic/ Physical Lab 2	2	Ch-306	Lab 2	2	Ch-406	Lab 2	2
Ch-108	Inorganic/Organic/Physical Lab 3	2	Ch-208	Inorganic/Organic/ Physical Lab 3	2	Ch-307	Lab 3	2	Ch-407	Lab 3/ 30 days Industrial training/ Research Training/ Internship*	2
Ch-109	Inorganic/Organic/Physical Lab 4	2	Ch-209	Inorganic/Organic/ Physical Lab 4	2	Ch-308	Lab 4 -	2	Comprehensive Viva-Voce**	2	2
	Total	26 Credits		Total	26 Credits		Total / 24 Credits				(50 marks)
	Total 700 marks			Total 700 marks			Total 600 marks				Total 600 marks

* Only for the students who have cleared all the subjects in the I & II semesters.

**Comprehensive Viva-Voce from all theory and practical subjects of all the four semesters.

Grand total = 700+700+600+600 = 2600 Marks.

Total credits: 100

Theory - 80 IA - 20 = 100

Lab - 35 IA - 15 = 50

SYLLABUS 2019-20

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 : **40 + Supernumerary seats + Payment seats= 60 (Total)**
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
Ch-101	Inorganic Chemistry I	4	52	3	80	20	100	4
Ch-102	Organic Chemistry I	4	52	3	80	20	100	4
Ch-103	Physical Chemistry I	4	52	3	80	20	100	4
Ch-104	Analytical Chemistry	4	52	3	80	20	100	4
Ch-105	Mathematics for Chemists (Soft Core)	3	36	3	80	20	100	2
Ch-106	Practical-I Inorg/Org/Phy	4	60	4	35	15	50	2
Ch-107	Practical-II Inorg/Org/Phy	4	60	4	35	15	50	2
Ch-108	Practical-III Inorg/Org/Phy	4	60	4	35	15	50	2
Ch-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
Ch-201	Inorganic Chemistry-II	4	52	3	80	20	100	4
Ch-202	Organic Chemistry-II	4	52	3	80	20	100	4
Ch-203	Physical Chemistry-II	4	52	3	80	20	100	4
Ch-204	Spectroscopy-I	4	52	3	80	20	100	4
Ch-205	Green Synthesis / Photo Chemistry (Soft Core)	3	36	3	80	20	100	2
Ch-206	Practical-I Inorg/Org/Phy	4	60	4	35	15	50	2
Ch-207	Practical-II Inorg/Org/Phy	4	60	4	35	15	50	2
Ch-208	Practical-III Inorg/Org/Phy	4	60	4	35	15	50	2
Ch-209	Practical-IV Inorg/Org/Phy	4	60	4	35	15	50	2
Total marks/credits							700	26

Practical: 30 marks for experiment + 5 marks for Viva-Voce

IA : Marks based on Test + Assignment + Seminar + Records

Scheme for continuous evaluation

Theory (each paper)

Tests* : 20 marks

Total : 20 Marks

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

* There should be minimum marks of 8 to be scored out of 20 for getting eligibility to attend the final University examination.

Practicals: (each practical)

Test (1 Test) 15 marks

Total : 15 marks

QUESTION PAPER PATTERN

Semester I:

Sub: Chemistry

Time: 3 Hrs

Max. Marks: 80

Note: Answer question Number one and any **SIX** in the remaining.

1. Answer any **TEN** sub divisions from the following

(10x2=20)

- a)
- b)
- c)
- d)
- e)
- f)
- g)
- h)
- i)
- j)

2 to 9

(6x10=60)

2.

- a)
- b)
- c)

(5+5) or (6+4) or(3+3+4)

SEMESTER – I

Ch-101 INORGANIC CHEMISTRY- I

UNIT- I

13h

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-Pauling, Allred-Rochow and Mulliken, electronegativity and partial ionic character; Bonds- Multicenter, Synergic and Agostic bonding, Lattice energy; Born-Landé equation, Kapustinskii equation; Fajan's rules- polarizability and partial covalent character, radius-ratio rules-limiting radius ratios of trigonal, tetrahedral, octahedral and cubic. Structures of solids- NaCl , CsCl , ZnS (zinc blende and wurtzite), rutile(TiO_2), perovskite(CaTiO_3), fluorite and anti fluorite. Zintl ions, Molecular orbital theory: formation of sigma, pi and delta bonds, LCAO and MO diagrams of heteronuclear diatomic (CO , NO , HF and ICl) and triatomic molecules (CO_2 and NO_2).

UNIT- II

13h

Chemistry of main group elements- Boranes- nomenclature, synthesis, structure and bonding in boranes, styx code, carboranes- classification, structures of ortho, meta, para- $\text{C}_2\text{B}_{10}\text{H}_{12}$, Wades rules, Metallocarboranes- synthesis and structure of $[\text{Fe}(\eta^5\text{-C}_2\text{B}_9\text{H}_{11})_2]^{2+}$, $\text{Fe}(\eta^5\text{-C}_2\text{B}_9\text{H}_{11})(\eta^5\text{-C}_5\text{H}_5)$, $[\text{Mo}(\text{CO})_3(\eta^3\text{-C}_2\text{B}_9\text{H}_{11})]^{2+}$, synthesis, structure and bonding in borazine, phosphazenes- synthesis, structure and bonding in $(\text{PNCI}_2)_3$, S,N- compounds- S_4N_4 , S_2N_2 and polythiazyl.

Silicates: Principles of silicates structures, classification with examples-ortho, pyro, cyclo, ino, phyllo and tecto silicates, isomorphous replacement; zeolites- sodalite and pentasil units, synthesis and structures of ZSM-5, zeolite A, faujasite and their uses.

UNIT-III

13h

HSAB concept: Basis of HSAB concept, acid-base strength, hardness and softness, symbiosis, applications and limitations of HSAB concept; Acid- base concept in non-aqueous media, reactions in BrF_3 , N_2O_4 , anhydrous H_2SO_4 , $\text{CH}_3\text{CO}_2\text{H}$. Isopoly and heteropoly acids of W and Mo, preparations, properties, structure and applications.

Stereoisomerism- Chirality, optical activity- CD, ORD, Cotton effect, absolute configuration of metal complexes, magnetic circular dichroism and its uses.

UNIT-IV

13h

Metal clusters- factors favouring M-M bond, classification, synthesis, structure and bonding in $[\text{Re}_2\text{Cl}_8]^{2-}$. Metal carbonyl clusters- LNCC's and HNCC's. Electron counting in carbonyl clusters, Wades-Mingos and Lauher rules.

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. 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.

SUGGESTED BOOKS

1. Basic Inorganic Chemistry- F. A. Cotton, G. Wilkinson and P. L. Gaus; John Wiley and sons. Inc, 3rd edition (2004).
2. Advanced Inorganic Chemistry, F. A. Cotton and G. Wilkinson. 6th edition (1999).
3. Inorganic Chemistry, J. E. Huheey, E. A. Keiter and R. L. Keiter, IV edition Addison; Wesley (1993).
4. Inorganic Chemistry, D. F. Shriver, P. W. Atkins and C. H. Langford, V edition ELBS; Oxford University Press, (2010)
5. Chemistry of elements; N. N. Greenwood and A. E. Earnshaw, Butterworth, II edition Heinemann (1997).
6. Concise Inorganic Chemistry, J. D. Lee , V edition; (1996).
7. Essentials of nuclear chemistry, H. J. Arniker, 4th edition; NAIL publishers (2011) Chapters 1, 3 and 4.
8. Nuclear and Radio chemistry; G.Friedlander, J.W.Kennedy, ES Macias and JM Miller; 1981, Chapters 8 and 9.
9. Inorganic Chemistry, Gary. L. Miessler and Donald . A. Tarr 5th Edition; (2014).
10. Inorganic Chemistry CE Housecroft and A G Sharpe 4th edition, pearson (2012).

Ch-102: ORGANIC CHEMISTRY- I

UNIT-I

52 Hours

Nature of Bonding in Organic Molecules

13h

Delocalized chemical bonding: Conjugation, cross conjugation, resonance, Hyperconjugation, Tautomerism.

Aromaticity: Huckel's MO theory. HMO diagram for benzene. Huckel's rules of aromaticity. Aromatic systems with electron numbers other than six (including azulene, tropone, tropolone and annulenes). Anti-aromaticity. Aromaticity in benzenoids. Homo-aromaticity. Alternant and non-alternant hydrocarbons. Energy levels in odd and even-alternant hydrocarbons, energy levels for the benzyl cation, benzyl free-radical and benzyl carbanion. Mesoionic compounds. Heteroannulenes. Fullerenes: C-60.

Synthetic Molecular Receptors: Definition and significance. Structure and function of receptors with molecular clefts, molecular tweezers, receptors with multiple hydrogen bonding sites. Crown ethers, cryptates, cyclodextrins, cyclophanes, catenanes and rotaxanes, calixarenes, ionophores, and micelles.

UNIT-II

Reaction Mechanisms: Structure and Reactivity

13h

Reactive Intermediates: Generation, structure, stability and reactivity of carbocations, carbanions, carbon free radicals, carbenes. Non-classical carbocations. 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.

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.

Aliphatic substitution reactions:

Nucleophilic substitution reaction at a saturated carbon: S_N1, S_N2, and SET mechanisms. Effect of substrate structure, attacking nucleophile and leaving group. Neighbouring group participation by sigma and pi bonds. Anchimeric effect. Ambident nucleophiles and substrates.

Electrophilic substitution reaction at a saturated carbon: S_E1, S_E2, and S_Ei mechanisms. Effect of substrate structure, leaving group and solvent polarity on the reactivity.

UNIT-III

13 h

Stereochemistry

Projectional formulae: Fischer, Newman, Sawhorse and flying wedge projections - their interconversions for acyclic and cyclic compounds.

Conformational analysis: D/L, R/S and M/P conventions. Cahn-Ingold Prelog (CIP) sequence rules.

Optical isomerism: Elements of symmetry and chirality. Chirality in compounds with a stereogenic centre. Center of chirality, axis of chirality, plane of chirality and helicity. Stereochemistry of allenes, alkylidene cycloalkanes and spiranes (with a stereogenic axis), biphenyls, cyclophanes, ansa compounds, *trans*-cyclooctene, helicenes, benzphenanthrenes. Configurational nomenclature.

Conformational analysis: Conformational analysis of cycloalkanes: cyclobutane, cyclopentane, cyclohexanes (mono-substituted e.g., methyl, *iso*-propyl, *tert*-butyl) and di-substituted cyclohexanes e.g., dialkyl-, dihalo-, diols), and cycloheptane.

Nomenclature and conformations of fused rings and bridged ring systems.

Prochirality: Enantiotopic and diastereotopic atoms, groups and faces. [S_i/R_e]. Basics of Cram's and Prelog's rules of asymmetric induction.

UNIT-IV

Carbohydrates:

13 h

Introduction. Determination of configuration of the monosaccharides, conformational analysis of monosaccharides. Derivatives of monosaccharides: acetals, aminosugars, deoxysugars and ethers. Synthesis of aldonic-, aldaric- uronic- acids and alditols.

Structural elucidation of sucrose and maltose.

Structures of lactose, gentiobiose and meliobiose. Photosynthesis of carbohydrates.

Heterocyclic compounds:

Introduction. Nomenclature of simple and fused heterocyclic compounds: Hantzsch-Widman method. Structure, reactivity, synthesis and reactions of pyrazole, imidazole, oxazole, isoxazole, thiazole, isothiazole. Synthesis of pyrimidine, purine, indole, benzimidazole, benzoxazole and benzisoxazole and coumarins.

SUGGESTED BOOKS

1. Organic Chemistry, R T Morrison, R N Boyd and S K Bhattacharjee, VII edition, Pearson, (2018).
2. Organic Chemistry, J Clayden, N Greeves and S Warren, II edition, Oxford University Press, (2014)
3. Advanced Organic Chemistry – Reactions, Mechanism and Structure, J March, John Wiley (2008).
4. Advanced Organic Chemistry, F A Carey and R J Sundberg Plenum, (2000).
5. A Guide Book to Mechanism in Organic Chemistry, P Sykes, VI edition, Pearson, (2003).
6. Structure and mechanism of Organic Chemistry, C K Ingold, II Edition, CBS, (2016).
7. Principles of Organic Synthesis, III edition), R O C Norman and J M Coxon, Blackie Academic and Professional (Indian Reprint), (2012).
8. Stereochemistry, V R Dani, Asian Books, New Delhi, (2014).
9. Stereochemistry of Organic Compounds, D Nasipuri, III edition, New-Age International, (2018).
10. Organic Stereochemistry, M J T Robinson, Oxford University Press, (2005).
11. Stereochemistry of Carbon Compounds, E L Eliel, S H Wilen and L N Mander, John Wiley, (1994).
12. Stereochemistry at a Glance J Eames, J M Peach, Blackwell, Oxford, (2003).
13. Heterocyclic Chemistry at a Glance, II edition, J A Joule and K Mills, Wiley, New York, (2012).
14. Organic Chemistry, Volume I, I L Finar, VI edition, Pearson, (2018).
15. Organic Chemistry, Volume II, I L Finar, VI edition, Pearson, (2018)

Ch-103 PHYSICAL CHEMISTRY- I

UNIT-I

13h

Quantum Mechanics-I

Introduction to quantum mechanics. Schrödinger wave equation. Time-independent and time dependent Schrödinger wave equations and the relation between their solutions. Eigen functions and Eigenvalues. Physical Interpretation of wave function. Concepts of Operators: Laplacian, Hamiltonian, Linear and Hermitian 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. Eigen functions and eigenvalues of angular momentum. Ladder operator method for angular momentum.

UNIT-II

13h

Quantum Mechanics-II

Schrödinger equation to hydrogen atom in spherical polar co-ordinates. Solution of ψ , ϕ , 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), spinorbital, anti symmetry and Pauli-exclusion principle, Slater determinants. Coupling of Angular momenta, Russell-Saunders and JJ-coupling, Atomic 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

13h

Chemical Dynamics-I

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

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.

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.

UNIT-IV

13h

Chemical Dynamics-II

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.

Unimolecular reactions: Perrin theory, Lindemann theory, and Hinshelwood theory.

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.

SUGGESTED BOOKS

1. Physical Chemistry- P. Atkins and J. D. Paula, 9th Edn., Oxford University Press (2010).
2. Physical Chemistry: A Molecular Approach, D. A. McQuarrie and Simon, Viva, New Delhi, (2003).
3. Introduction to Quantum Chemistry, A. K. Chandra, 3rd Edn. Tata McGraw Hill, (1991).

4. Quantum Chemistry, Ira. N. Levine, Prentice Hall, New Jersey, (1991).
5. Quantum Chemistry, R. K. Prasad, New Age International, 4thEdn., (2010).
6. Quantum Mechanics by G R Chatwal and S K Anand, Himalaya Publications, 8thEdn, 2012.
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 of Chemical Transformations- J. Rajaraman and J. Kuriakose, Mc Millan India Ltd. (2011).
10. Biochemistry, - Geoffrey Zubay, 2nd Edn., Macmillan Publishing Co. New York (1988).
11. Physical Chemistry of Surfaces- A. W. Adamson, Wiley-Interscience Publisher Inc., New York (1997).
12. Introduction to surface chemistry and Catalysis by Gabor A. Somorjai and Yimin Li, John 2ndEdn. Wiley and Sons Ltd, Hoboken, United States, 2010.

Ch-104 Analytical Chemistry

13 h

UNIT – I Basic concepts

Practicing safety measures in chemical laboratories, Fire hazards, toxic chemicals: Acids/bases/solvents handling, storage, dilution, disposal of chemicals, acid/ solvent bottles etc. toxic chemicals sampling and handling hazards, safety data sheets, miniaturization of analytical instruments, their significance in modern chemical analysis.

Preparation of dilute acids from concentrated/fuming acids like H_2SO_4 , handling liquid bromine, elemental mercury, solvent ether, liquor ammonia and other chemicals.

Errors in chemical analysis: absolute, relative error, random error distribution, Gaussian curve, Limitations of analytical methods, determinate and indeterminate errors, minimization of errors. Accuracy and precision, distribution of random errors, the normal error curve. Statistical treatment of finite samples - measures of central tendency and variability: mean, median, range, standard deviation, variance, confidence limits. Comparison of an experimental mean and a true mean. F-test, rejection of result - Q-test, Student's t-test, numerical problems.

UNIT-II Quantitative Analysis-Classical methods

13 h

Classification of analytical methods, types of instrumental analysis, factors influencing choice of analytical method, qualitative and quantitative analysis, Units used in chemical analysis, their conversion, ppm, ppb, ppt etc.

Titrimetry

Acid-Base: Theory of indicators, Ex: Phenol-phthalien, Methyl red. Titration curves for mono functional acid and base, pH calculations, fractions of phosphoric acid species as a function of pH. Titration curves for H_3PO_4 .

Complexometry: Theory of metal ion indicators, 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, effect of pH

and nature of titration curve. Masking and demasking, type of EDTA titrations, titrations involving monodentate bidentate and polydentate ligands.

Redox: Mechanism of indicator action, criteria for the selection of indicators. Feasibility of redox titration. Titration of multicomponent system, Nernst equation. Applications: Oxidants such as Ce(IV), bromate, Iodates.

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

Gravimetry

Quantitative precipitation, *Precipitation from Homogeneous Solution (PFHS)*, Formation and treatment of precipitates, co-precipitation, post precipitation. Conditions for precipitation, washing, drying and igniting the precipitates. Important precipitating agents such as DMG, oxine, thiocyanate and their significance in inorganic analysis, errors in gravimetric analysis.

Unit-III – Quantitative Analysis – Instrumental methods(Spectroscopy)

13 h

Electromagnetic radiation, interaction with matter, absorption, Beer-Lambert's law, derivation, molar absorptivity, Sandell sensitivity, Ringbom plot, deviations, limitations, Calibration with standards, standard addition, internal standard addition, limit of detection, limit of quantification, Instrumentation, radiation sources, wavelength selection devices, optical slits, single beam and double beam instruments, photo electric colorimeter, scanning devices, merits and limitations, numerical problems on application of Beer's law.

Unit IV- Separation Methods

13 h

Solvent Extraction – Types, batch, continuous, efficiency, selectivity, Distribution coefficient, Nernst distribution law, derivation, factors affecting the partition, applications. Chromatography – Types, Terminology, Principles of paper, thin layer, column, gas chromatography, column efficiency, plate theory, factors affecting the column efficiency, band broadening, R_f factor, Van-Deemter equation, medium performance liquid chromatography, high performance liquid chromatography, reserved phase liquid chromatography, super critical fluid chromatography, characteristics of super critical fluids, 2D-thin layer chromatography, electrophoresis, principles, applications etc. numerical problems on solvent extraction, R_f factor and van Demeter equation.

Suggested books:

1. Fundamental of Analytical Chemistry, D.A. Skoog, D.M. West, Holler and Crouch, 8th edition, Saunders College Publishing, New York, 2005.
2. Analytical Chemistry, G.D. Christian, 6th edition, John Wiley & Sons, Inc, India, 2004.
3. Quantitative Analysis, R.A. Day and A.L. Underwood, 6th edition, Prentice Hall, Inc. New Delhi, 1993
4. Vogel's Textbook of Quantitative Chemical Analysis, J. Mendham, R.C. Denney, J.D. Barnes and M.J.K. Thomas, 6th edition, Third Indian Reprint, Pearson Education Pvt. Ltd., New Delhi, 2003.
5. Analytical Chemistry Principles, John H. Kennedy, 2nd edition, Saunders College Publishing, California, 1990.
6. Principles and Practice of Analytical Chemistry, F.W. Fifield and Kealey, 3rd edition, Blackwell Sci., Ltd. Malden, USA, 2000.
7. Modern Analytical Chemistry, David Harvey, McGraw Hill, New Delhi, 2000.
8. Practical Volumetric Analysis, Peter A C McPherson, RSC, Cambridge, UK, 2015.
9. Analytical Chemistry for Technicians, John Kenkel, 4th edn. CRC Press, London, 2014.
10. Undergraduate Instrumental Analysis, J.W. Robinson, E.M. Skelly Frame, G. M. Frame II, 6th edn. Marcel Dekker, New York, 2009.

Ch-105 MATHEMATICS FOR CHEMISTS

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.

Ch-106/ PRACTICAL –I INORGANIC/ORGANIC/PHYSICAL

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, Zr, V and Li.

C-107 Inorganic chemistry practical-II

Preparation of inorganic complexes:

1. Cis- potassium dioxalatodiaquachromium(III) complex.
2. Hexamminecobalt(III) chloride.
3. Mercury tetrathiocyanatocobaltate.
4. Pentamminechlorocobalt(III) chloride.
5. Potassium tris(oxalato)ferrate trihydrate.
6. Potassium tris(oxalato)aluminate trihydrate.

C-108 Inorganic Chemistry Practical-III

Gravimetric analysis

1. Determination of Fe in iron ore as Fe_2O_3 .
2. Determination of Ni as nickel dimethylglyoximate in Cu and Ni solution.
3. Determination of Ca as $CaC_2O_4 \cdot H_2O$.
4. Determination of Al as aluminiumoxinate.
5. Determination of Cu as $CuSCN$ in Cu and Fe solution.
6. Determination of Zn as $ZnNH_4PO_4$.

C-109 Inorganic Chemistry Practical-IV

Volumetric analysis

1. Determination of Ca and Mg in Dolomite solution using EDTA.
2. Determination of Cu in Cu and Ni solution iodometrically.
3. Determination of Fe in Cu and Fe solution (using $K_2Cr_2O_7$).
4. Determination of Cr and Fe in a mixture using ceric ammonium sulphate.
5. Determination of Fe and Al in mixture using EDTA.
6. Determination of percentage of Fe and oxalate in $K_3Fe(C_2O_4)_3 \cdot 3H_2O$

Suggested Books:

1. Vogel's Text book of Qualitative Chemical Analysis, J. Bassett, G. H. Jeffery and J. Mendham, 7th edition, ELBS (2013).
2. Vogel's text book of Quantitative Chemical Analysis, 6th Edition, J. Bassett, G. H. Jeffery and J. Mendham, and R. C. Denny, J D Barnes, M. Thomas Prentice Hall (2000)
3. Inorganic Semimicro Qualitative Analysis, V. V. Ramanujam; The National Pub. Co. (1990).
4. Practical Inorganic Chemistry, G. Marr and B. W. Rockett, Von Nostrand Reinhold Co., London (1972).
5. An Advance course in practical chemistry, A Ghoshal, B Mahapatra and A K Nad; New central book agency Pvt.Ltd. 3rd edition 2007.
6. Advanced inorganic analysis, S K Agarwal and Keemtilal; Pragati prakashan, 12th edition 2014.

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

Ch-106 Organic Chemistry Practical-I

Preparation (one stage)

1. Oxidation of cyclohexanol.
2. Preparation of S-benzylisothiuroniumchloride.
3. Synthesis of picric acid.
4. Synthesis of glucose pentaacetate.
5. Synthesis of 2,4,6-tribromoaniline.
6. Cannizarro reaction: benzaldehyde to benzyl alcohol and benzoic acid.
7. Dehydration of cyclohexanol to cyclohexene.
8. Claisen-Schmidt reaction: benzaldehyde and acetone to dibenzalacetone.
9. Sandmeyer reaction: 4-chlorotoluene from 4-toluidine.
10. Pechmann reaction: resorcinol and ethylacetoacetate to 7-hydroxy-4-methylcoumarin
11. Synthesis of 2,4-dichlorophenoxyacetic acid.
12. Synthesis of resacetophenone from resorcinol.

Ch-107 Organic Chemistry Practical-II

Qualitative analysis

Systematic analysis and identification of bifunctional organic compounds.

Ch-108 Organic Chemistry Practical – III Preparation (Two and three stages)
4-Nitroaniline from acetanilide

1. 4-Bromoaniline from acetanilide.
2. 3-Nitrobenzoic acid from benzoic acid/methyl benzoate.
3. 2,4-Dinitrophenylhydrazine from chlorobenzene.
4. N-Methylantranilic acid from phthalic acid.
5. Benzanilide from benzophenone.
6. Benzilic acid from benzoin.
7. Synthesis of acridone.
8. Synthesis of hydantoin.
9. Anthracene to anthrone
10. Succinic acid to N-bromosuccinimide.
11. Maleic acid to dimethylacetylenedicarboxylate.

Ch-109 Organic Chemistry Practical-IV

Quantitative analysis

1. Titrimetric estimation of mono-, dicarboxylic-, amino- and aryloxyacetic acids.
2. Estimation of carboxylic acid in presence of an amide/ester.
3. Saponification value of oil.
4. Estimation of glucose by Fehling's method/Bertrand's method.
5. Estimation of keto-group.
6. Estimation of phenols.
7. Iodine value of oil (Chloramine-T method) Acid and ester, acid and amide in the mixture of two.

SUGGESTED BOOKS

1. Vogel's Text Book of Practical Organic Chemistry – V edition, B. S. Furniss, A. J. Hannaford, P. W. G. Smith and A. R. Tatchell - Pearson, (2003).
2. Laboratory manual of Organic Chemistry- B. B. Dey, M. V. Sitaraman and T.R. Govindachari, Allied Publishers, New Delhi, (1996).
3. Practical Organic Chemistry, IV edition, – F. G. Mann and B. C. Saunders, - Pearson, 2009).
4. Text Book of Practical Organic Chemistry including qualitative analysis – IV Edition, A. I. Vogel and A. R. Tatchell, Longman, London, (1996).
5. Test Book of Quantitative Organic Analysis- A. I. Vogel, (1996).
6. A Handbook of Organic Analysis – Qualitative and Quantitative – IV Edition, H. T. Clarke, Hodder and Staughton, New Delhi (2017).
7. Comprehensive practical organic chemistry: Preparation and quantitative Analysis, V. K. Ahluwalia, R. Aggarwal, Universities Press (India), 2000.
8. Comprehensive practical organic chemistry: Qualitative analysis, V. K. Ahluwalia, S. Dhingra, Universities Press (India), 2000.
10. An advanced course in practical chemistry, A. Ghoshal, B. Mahapatra and A.Kr. Nad, New central book agency, Calcutta, 2000.
11. Advanced practical organic chemistry, J. Mohan, Vol. I and II, Himalaya Publishing House, 1992.
12. Practical organic chemistry (Quantitative analysis), B. B. Dey, M. V. Sitaraman and T. R. Govindachari, Allied Publishers, New Delhi, 1992.
13. Advanced Practical Organic Chemistry, III Edition, J. Leonard, B. Lygo and G. Procter, CRC Press, Routledge, (2013).
14. Qualitative Organic Analysis – Spectrochemical Techniques W. Kemp, II edition, Mc-Graw Hill, London, (1986).

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

C-106 Physical Chemistry Practical -I

1. Study of Acid catalysed hydrolysis of methyl acetate at lab temperature and reporting the calculated and graphical rate constants
2. Determination of Velocity constant for the saponification of Ethyl acetate at lab temperature and comparing it with graphical value.
3. Verification of Beer's Law: Colorimetric estimation of Cu^{2+} ions and reporting the Molar extinction coefficient.
4. Determination of heat of solution of a sparingly soluble salt.
5. Colorimetric estimation of Fe^{2+} ions in a given solution by titrating FAS versus KMnO_4 solution.
6. Study of kinetics of the reaction between KI and $\text{K}_2\text{S}_2\text{O}_8$ solution.
7. Construction of phase diagram of two component systems and determination of E_c , E_T and the Composition of given unknown.
8. Determination of partial molar volume of solute – water system by apparent molar volume method.
9. Analysis of a binary mixture by viscosity measurement 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 of lithium sulphate versus BaCl_2 and reporting the concentration of Li_2SO_4 .
2. Determination of concentration of a weak acid by titrating against a weak base.
3. Determination of a dissociation constant of weak acid (CH_3COOH).
4. Determination of Equivalent conductance of a given strong electrolyte.
5. Determination of the concentration of a strong acid and a salt in a given mixture of by titrating against a 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 and estimation of the concentration of AgNO_3 .
9. Determination of pK_a and K_a values of the weak acid by titrating against a strong base using quinhydrone electrode.
10. Determination and comparison of pH values of buffer solutions by using quinhydrone electrode and glass electrode.

C-108 Physical Chemistry Practical -III

1. Study of acid hydrolysis of methyl acetate for two different concentrations of HCl and reporting the relative strength.
2. Study the hydrolysis of methyl acetate in the presence of HCl at two different temperatures and reporting 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 and determination of the constants A and B.
7. Analysis of a binary mixture of two miscible liquids by surface tension method
8. Construction of phase diagram of Urea - KCl - H_2O system.
9. Determination of heat of neutralization of two acids and their relative strength.
10. Evaluation of Arrhenius parameter for the reaction between $\text{K}_2\text{S}_2\text{O}_8$ versus KI (first order)

C-109 Physical Chemistry Practical -IV

Conductometry

1. Determination of concentration of mixture of strong acid and weak acid versus strong base.
 2. Determination of concentration of Weak acid with salt versus strong base.
 3. Determination of strength of a strong acid, weak acid and a salt versus strong base
- pH metry
5. Determination of the acidic and basic dissociation constant and isoelectric point of an amino acid by pH metry.

6. Determination of pKa value or Dissociation constant of phosphoric acid.
 7. Determination of pH of acetic acid with sodium acetate buffer.
- Potentiometry
8. Determination of concentration and amount of $K_2Cr_2O_7$ by titrating against FAS and calculation of redox potential.
 9. Determination of concentration of mixture of acids by titrating against NaOH solution.
 10. Determination of concentration of $KMnO_4$ by titrating against FAS and calculation of redox potential.

SUGGESTED BOOKS

1. Advanced Practical Physical Chemistry by J. B. Yadav, Goel Publications, Meerut (2012).
2. Senior Practical Physical Chemistry by B. C. Kosla, Simla Printers, New Delhi (1987).
3. Experimental Physical Chemistry by Daniel et al., McGraw Hill, New York (1962).
4. Practical Physical Chemistry by A.M James and P. E. Pritchard, Longman's Group Ltd (1968).
5. Experimental Physical Chemistry by Wilson, Newcombe & others, Pergamon Press, New York (1962).
6. Experimental Physical Chemistry by R. C. Behra and B Behra, Tata McGraw, New Delhi (1983).
7. Experimental Physical Chemistry by V. D. Atavale and Parul Mathur, New Age International, New York (2001).
8. Practical's in physical chemistry A. Modern Approach by P.S Sindhu, Mac. Millan Publishers, Delhi (2006).

II SEMESTER

Ch-201: INORGANIC CHEMISTRY- II

UNIT-I

13h

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- hydride, dihydrogen, dioxygen, isocyanide, N_2 and tertiary phosphine complexes of transition metals, metal carbonyls-terminal and bridge carbonyls, detection, metal nitrosyls- terminal (linear and bent) and bridge.

UNIT-II

13h

Metal- ligand bonding- Coordination numbers 3 to 8. Crystal field theory, salient features, spectrochemical series, splitting of d-orbitals in tetrahedral, square planar, trigonal bipyramidal, square-pyramidal and octahedral geometry, applications of CFT- colors of transition metal complexes, magnetic properties of octahedral complex, Jahn Teller distortion, CFSE and their uses, factors affecting CFSE, limitations of CFT, experimental evidences 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 and its detection.

UNIT-III

13h

Electronic spectra of coordination compounds- Spectroscopic ground states, selection rules, term symbols for d^n ions, Racah parameters, Orgel, Correlation and Tanabe-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.

UNIT-IV

13h

Magnetic properties of coordination compounds- Types of magnetism, temperature effect, 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 metal complexes: Basic photochemical processes, Kasha's rule, quantum yield, Jablonskii diagrams, photo substitution reactions, photo-redox reactions, ligand photoreactions.

SUGGESTED BOOKS

1. Advanced 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, 2nd edition, Butterworth Heinemann (1997).
3. Inorganic Chemistry J. E. Huheey, E. A. Keiter and R. L. Keiter, 4th edition; Addison; Wesley (1993).
4. Inorganic Chemistry, D. F. Shriver, P. W. Atkins and C. H. Langford, 5th edition, ELBS; Oxford University Press, (2010)
5. Inorganic Electronic spectroscopy, A. B. P. Lever, 2nd edition, Elsevier. (1984).
6. Magnetochemistry, R.L. Carlin, Springer Verlag (1986).
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. Inorganic chemistry G L Miessler, P J Fisher and D A Tarr 5th edition (2008).

Ch-202 ORGANIC CHEMISTRY – II

UNIT-I

Reaction Mechanisms: Aromatic Substitution Reactions

13h

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 S_NAr , S_N1 , benzyne and S_N1 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

Reaction Mechanisms: Addition Reactions

13h

Addition to carbon-carbon multiple bonds: mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals. Regio-, stereo- and chemo- selectivities. 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

13h

Reaction Mechanisms: Elimination Reactions

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 and Name Reactions:

Carbon-carbon: Wagner-Meerwein, Pinacol-Pinacolone, Fries, Benzil-benzilic acid rearrangements, Wolff rearrangement and Arndt-Eistert reaction, Tiffeneau- Demjanov reaction, Fritsch-Buttenberg-Wiechell rearrangement. Favorskii rearrangement, Dienone-phenol rearrangement, Baker-Venkataraman rearrangement.

Carbon-nitrogen: Beckmann-, Hofmann-, Curtius-, Lossen- and Schmidt-rearrangements. Stevens-, Neber- rearrangement. Benzidine rearrangement.

Carbon-oxygen: Wittig rearrangement, Baeyer-Villiger oxidation.

Chemistry of biological molecules - II**Amino acids and Peptides**

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.

Vitamins

Introduction. Biological importance and synthesis of Vitamins A, Vitamin B₁ (thiamine), Vitamin B₆ (pyridoxine), folic acid, pantothenic acid, riboflavin, Vitamin C, Vitamin E (α -tocopherol), Vitamin H (biotin), Vitamins K₁ and K₂.

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, (2000).
3. A Guide Book to Mechanism in Organic Chemistry, P Sykes, VI edition, Pearson, (2003).
4. Structure and Mechanism of Organic Chemistry, C. K. Ingold, II Edition, CBS, (2016).
5. Organic Chemistry, R T Morrison, R N Boyd and S K Bhattacharjee, VII edition, Pearson, (2018).
6. Principles of Organic Synthesis, III edition), R O C Norman and J M Coxon, Blackie Academic and Professional (Indian Reprint), (2012).
7. Natural Products: their chemistry and biological significance, J Mann, Longman, (2000)
8. Organic Chemistry, Volume I, I L Finar, VI edition, Pearson, (2018).
9. Organic Chemistry, Volume II, I L Finar, VI edition, Pearson, (2018).
10. Organic Chemistry, J Clayden, N Greeves and S Warren, II edition, Oxford University Press, (2014)
11. Name Reactions – A collection of detailed reaction mechanisms, J J Li Springer, (2012)
12. Modern Methods of Organic Synthesis W Carruthers and I Coldham, IV edition, Cambridge University Press, (2015).
13. Peptides Chemistry: A practical text book, M. Bodansky, Springer-Verlag NY, (1988).
14. Solid-phase peptide synthesis: A practical Approach-E. Artherton & R.C. Sheppard, I R L, Oxford Univ. Press, (1989).
15. Peptides: Chemistry and Biology, N Selwad and H.-D. Jakubke, Wiley-VCH, (2002).

203: PHYSICAL CHEMISTRY- II

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-DuhemMargulus 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 nonideal system-Excess thermodynamic function, GE, SE, HE 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 Cv) 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. Comparison of Bose-Einstein and Fermi-Dirac statistics with Maxwell – Boltzmann statistics. Problems and their Solutions. Non-equilibrium Thermodynamics : Thermodynamic criteria for non-equilibrium 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. deDonder'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

Electrochemistry-I

13h

Electrochemistry of solutions: Ionic atmosphere, Debye-Huckel theory for the problem of activity coefficient, Debye-Huckel limiting Law, Debye-Huckel equation for appreciable concentration, Debye-HuckelOnsagar conductance equation and its extension to ion solvent interactions, 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: Helmholtz theory, Guoy- Chapman theory, Stern model. Overpotential: Concentration, activation and ohmic overpotential; Derivation of Butler- Volmer equation.

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

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 technique-Principle, BME- Merits and limitations, experimental, polarogram, half wave potential, diffusion controlled current, Ilkovic equation (no derivation), qualitative and quantitative estimation of metal ions.

Advanced Electrodes: Rotating disc electrodes, Membrane electrodes (Definition, examples with diagrams and applications to each), carbon electrodes.

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. Elements of Classical and Statistical Thermodynamics, L. K. Nash, Addison-Wiley (1979).
6. Thermodynamics, Statistical Thermodynamics and Kinetics by Thomas Engel & Philip Reid, Pearson Education inc. (2007).
7. Modern Electrochemistry Vol-1 and 2, J. O. M. Bockris and A. K. N. Raddy, Plenum, New York (1978).
8. An introduction to electrochemistry: Samuel Glasstone East-West, edition New Delhi (1942)
9. 10. Text book of physical chemistry Samuel Glasstone, 2nd edition, Mac Millan India Ltd (1991)
10. Principles and applications of Electrochemistry- D. R. Crow 3rd edition, Chapmanhall London (1988).
11. Physical chemistry through problems by S K Dogra and S Dogra, Wiley Eastern Ltd., 4th Edn. 1993.
12. Electrochemical methods by A J Bard and I R Faulkner, 2nd Edn., Wiley New York, 2000.

UNIT-I

Symmetry and Group Theory in Chemistry

13h

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

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

UNIT-II

13h

Infrared Spectroscopy-I

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.

Infrared Spectroscopy-II

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

UNIT-III

13h

Raman Spectroscopy

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 asymmetric 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

Microwave Spectroscopy

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

UNIT – IV

Electronic Spectroscopy

13h

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).

Ch-205 GREEN SYNTHESIS (SOFT CORE)

36 Hours

UNIT-I

Use of ultrasound and Microwaves in organic Synthesis

12 h

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.

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

UNIT-II

Polymer supported reagents in organic synthesis

12 h

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

Substrate covalently bound to the support: Synthesis of oligosaccharides, Dieckmann cyclisation. Preparation of polymer bound aldehyde and application in aldol and Wittig reactions. Synthesis of polystyrylboronic 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.

Phase transfer catalysis and Crown ethers

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-III

Multi-component Reactions

12 h

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-Hilman; Petasis; Ivanov and Suzuki coupling reaction.

SUGGESTED BOOKS

1. Some modern methods of Organic Synthesis, W. Caruthers, Cambridge Univ. Press London, 2nd Edition, 1998.
2. Organic synthesis: Special techniques, V. K. Ahluwalia and R. Aggarwal, Narosa, New Delhi, 2003.
3. Green Chemistry, environment friendly alternatives, R. Sanghi and M. M. Srivastava, Narosa, New Delhi, 2003
1. Green Chemistry-an introductory text, M. Lancaster, Royal Society of Chemistry, UK, 2003.
2. Organic chemistry Vol. 2, 6th Edition, I. L. Finar, Longman, 1992.
3. Crown ethers & cryptands, G. W. Gokel, Royal Society of Chemistry, UK, 1991.
4. Macrocyclic Polyether Chemistry, G. W. Gokel, S. M. Korzeniowski, Vol 1 to3, Wiley, NY, 1978, 1981, 1987.
5. Phase Transfer Catalysis in Organic Synthesis, W. B. Weber, G. W. Gokel, Springer, Berlin, 1977.
6. Phase Transfer Catalysis, E. V. Dehmlov, S. S. Dehmlov, 2nd Edn., Verlag chemie, Wienheim, 1983.
7. Polymers as aids in Organic synthesis, N. K. Mathur, C. K. Narang and R.E. Williams, Academic Press, NY, 1980.

Ch -205 PHOTO CHEMISTRY (SOFT CORE)

UNIT-I

12h

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.

UNIT-III

12h

Photosensitized reactions: photodissociation-Gas phase photolysis, photofragmentation in liquid phase, photodegradation of polymers, Isomerization and other rearrangement reactions, Atmospheric photochemistry.
Photoelectrochemistry: Introduction, efficiency of conversion of light to chemical and electrical energy, frequently measured quantities. Photosplitting of water using colloidal suspensions.
Semi conductors: Bonding, 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.
Photocatalysis: Photocleavage of environmentally hazardouswaste matter by using TiO₂, ZnO and MgO. Photooxidation and photoreduction reactions.

SUGGESTED BOOKS

1. Fundamentals of photochemistry, K.K. RohatgiMukherjee, 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 (1st 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, John Wiley & Sons Inc. (1975).
7. Physical Chemistry, P. W. Atkins, Julio de Paulo ELBS 7th Edition (2002)

**Ch- 206, Ch- 207, Ch- 208 and Ch-209
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.