

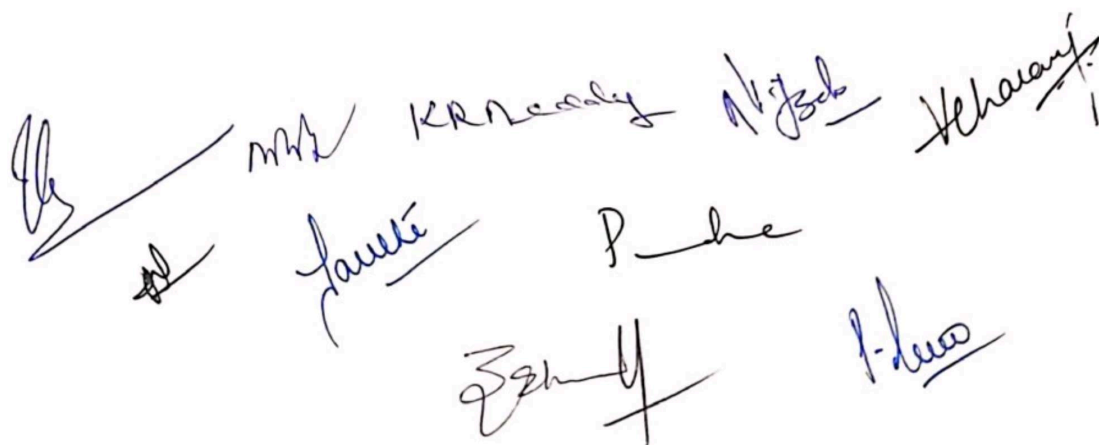
DEPARTMENT OF CHEMISTRY
OSMANIA UNIVERSITY
 (Effective from academic year 2023-2024 for Campus, Constituent and
 Affiliated colleges)

Semester I

	Hrs. /week	internal assessment	Semester exam	Total	Credits
CH101T (*)	3	30 marks	70 marks	100 marks	3
CH102T (*)	3	30 marks	70 marks	100 marks	3
CH103T (*)	3	30 marks	70 marks	100 marks	3
CH104T (*)	3	30 marks	70 marks	100 marks	3
CH151P (IC LAB*)	4			50 marks	2
CH152P (OC LAB*)	4			50 marks	2
CH153P (PC LAB*)	4			50 marks	2
CH154P (AC LAB*)	4			50 marks	2
Total				600 marks	20

Semester II

	Hrs. /week	internal assessment	Semester exam	Total	Credits
CH201T (*)	3	30 marks	70 marks	100 marks	3
CH202T (*)	3	30 marks	70 marks	100 marks	3
CH203T (*)	3	30 marks	70 marks	100 marks	3
CH204T (*)	3	30 marks	70 marks	100 marks	3
CH251P (IC LAB*)	4			50 marks	2
CH252P (OC LAB*)	4			50 marks	2
CH253P (PC LAB*)	4			50 marks	2
CH254P (ACS LAB*)	4			50 marks	2
Total				600 marks	20



M.Sc. CHEMISTRY SYLLABUS

(Effective from academic year 2023-2024 for Campus, Constituent and Affiliated colleges)

SEMESTER – I

Semester-I and Semester-II syllabus is common for all specializations i.e., Inorganic, Organic, Physical, Physical- Organic, Analytical and Pharmacoinformatics.

Paper 1: CH 101 (Inorganic Chemistry)

IC 01: Symmetry of molecules

IC 02: Bonding in Metal Complexes-I

IC 03: Coordination equilibria

IC-01: Symmetry of Molecules:

15 hrs

Symmetry Operations and Symmetry Elements: Rotational axis of symmetry and types of rotational axes, plane of symmetry and types of planes, improper rotational axis of symmetry, inversion center and identity element. Molecular Point Groups: Definition and notation of point groups. Classification of molecules based on molecular point groups. Systematic assignment of point groups to molecules (flow chart). Exercises in molecular point groups: C_1 , C_s , C_i , C_n , C_{nv} , C_{nh} , $C_{\infty v}$, D_n , D_{nh} , D_{nd} , $D_{\infty h}$, S_n (n =even), T_d (CH_4 , SiH_4), O_h (SF_6), I_h ($B_{12}H_{12}^{2-}$), K_h . Descent and ascent in symmetry with substitution (eg. NH_3 , CH_4 , PCl_5 , ML_6). Symmetry restrictions on dipole moment. Symmetry criteria for optical activity.

IC – 02: Bonding in metal complexes – I:

15 hrs

Crystal Field Theory: Salient features of CFT. d-orbital splitting patterns in regular octahedral, tetrahedral, square planar, tetragonally distorted octahedral, Jahn-Teller theorem, trigonal bipyramidal, trigonal planar, pentagonal bipyramidal, and linear geometries. Factors influencing magnitude of Δ_o . Concept of weak field and strong fields. Calculation of crystal field stabilization energies (CFSE's) in six and four coordinate complexes. Applications of CFSE-normal and inverse spinels.

Magnetic properties of transition metal complexes: Types of magnetic behavior. Magnetic susceptibility. Calculation of magnetic moment from magnetic susceptibility. Spin only formula. Quenching of orbital angular momentum. Determination of magnetic moment from Guoy's method. Applications of magnetic moment data for the determination of oxidation states, bond type and stereochemistry. Spin crossover.

IC-03: Coordination Equilibria:

15 hrs

Solvation of metal ions. Metal complex formation in solution. Binary metal complexes. Stability constants: Types (concentration, Thermodynamic and Conditional), stepwise and overall stability constants and relationships between them. Factors influencing the stability constants - (i) Metal ion effects: charge, size, charge/size IP, crystal field effect (Irving-William's order of stability), Jahn-

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Teller effect. (ii) Ligand effects: Basicity, substituent effect, steric, chelate (size and number of chelate rings), macrocyclic and cryptate effects (crown ethers, cryptands, size match selectivity or concept of hole size and its limitations), macrocycles with pendent groups. Pearson's theory of hard and soft acids and bases (HSAB): Principle and applications. Methods used for the determination of stability constants: pH metric, spectrophotometric and polarographic methods. Ternary metal complexes: Definition, formation of ternary metal complexes, step-wise and simultaneous equilibria with simple examples.

References

1. Chemical applications of group theory, F Albert Cotton, 3rd Edition, Wiley India (2009).
2. Symmetry and Spectroscopy of Molecules, K.Veera Reddy, New Age Int. (P) Ltd. (2002)
3. Symmetry in chemistry, Hans H Jaffe, Milton Archin, Dover publications Inc (2002)
4. Molecular symmetry and group theory, Allen Vincent, 2nd Edition, John Wiley & sons Ltd. (2010)
5. Advanced Inorganic Chemistry, F.A.Cotton & G.Wilkinson, 3rd Edition, Wiley Interscience Publications (1972).
6. Advanced Inorganic Chemistry. F.A.Cotton, G.Wilkinson, C.A.Murillo & M.Bochmann, 6th Edition, Wiley Interscience Publications N.Y (1999).
7. Inorganic Chemistry, J.E. Huheey, K.A.Keiter and R.L.Keiter, 4th Edition, Harper Cottens College Publications (1993).
8. Inorganic Chemistry, Keith F.Purcell and John C.Kotz, Holt-Saunders Int. Edn.London (1977).
9. Principles of Inorganic Chemistry, Puri, Sharma, Kalia, 33rd Edition, Vishal Publications (2022).
10. Metal complexes in Aqueous Solutions, A.E Martell and Robert Hancock, Springer Science (1996)

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Paper-II: CH 102 (Organic Chemistry)

OC-01: Stereochemistry

OC-02: Reaction mechanism-I

OC-03: Conformational analysis (Acyclic systems)

OC-01: Stereochemistry

15 hrs

Molecular representations: Wedge, Fischer, Newman and Saw-horse formulae, their description and interconversions.

Molecular Symmetry & Chirality: Symmetry operations and symmetry elements (C_n & S_n). Criteria for Chirality. Desymmetrization.

Axial, planar and helical chirality: Axially chiral allenes, spiranes, alkylidene cycloalkanes, chiral biaryls, atropisomerism, buttressing effect, planar chiral ansa compounds and trans-cycloalkenes (upto cyclodecene and their methyl analogues), helically chiral compounds and their configurational nomenclature

Relative and absolute configuration: Determination of configuration by chemical correlation methods.

Racemisation and resolution techniques: Racemisation; mechanism Via carbocation, carbanion and free radical. Resolution by direct crystallization, diastereoisomer salt formation chiral chromatography and asymmetric transformation.

Determination of configuration in E, Z-isomers: Spectral and Chemical methods of configuration determination of E,Z isomers. Determination of configuration in aldoximes and ketoximes.

OC-02: Reaction mechanism-I

15 hrs

Determination of reaction mechanism: Introduction: product isolation, isolation, detection and trapping of intermediates, addition of suspected intermediate-von Richter rearrangement. Use of isotopes, isotope effects, and crossover experiments. Use of IR and NMR in the investigation of reaction mechanism

Electrophilic addition to carbon carbon double bond: Stereoselective addition to carbon carbon double bond; *anti* addition: Bromination and epoxidation followed by ring opening. *Syn* addition : OsO_4 and $KMnO_4$.

Elimination reactions Elimination reactions E_2 , E_1 , E_1cB mechanisms. Orientation and stereoselectivity in E_2 eliminations. Pyrolytic *syn* elimination and α -elimination, elimination Vs substitution.

Nucleophilic Aromatic substitution: Aromatic Nucleophilic substitution: $S_N1(Ar)$, $S_N2(Ar)$, and benzyne mechanisms and evidence.

OC-03: Conformational analysis (acyclic systems)

15hrs

Conformational isomerism: Introduction to the concept of dynamic stereochemistry. Conformational diastereoisomers and conformational enantiomers. Conformational nomenclature: Conventional method, limitations, Klyne-Prelog terminology. Study of conformations in, dihaloethanes, halohydrin, ethylene glycol, 2,3-dihalobutanes, butane-2, 3-diol, amino alcohols

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and 1,1,2,2-tetrahalobutanes.

Conformations of unsaturated acyclic compounds: Propylene, Acetaldehyde and Butanone

Physical methods for conformational Analysis: Use of dipole moment, UV, IR and NMR, spectral methods in conformational analysis.

Conformational affects on the stability and reactivity of acyclic diastereoisomers: Steric and stereoelectronic factors-examples. Conformation and reactivity (E2 eliminations, NGP, Stereochemistry-Rearrangements). The Curtin – Hammett principle.

References

1. Stereochemistry of carbon compounds by Ernest L. Eliel and Samuel H. Wilen
2. Stereochemistry of organic compounds- Principles and Applications by D. Nasipuri
3. Advanced Organic Chemistry by Jerry March
4. Mechanism and Structure in Organic Chemistry S. Mukerjee
5. Organic chemistry by Jonathan Clayden, Nick Greeves and Stuart Warren
6. Organic Reactions and their mechanisms by P.S. Kalsi
7. Stereochemistry: Conformation & Mechanism by P S Kalsi

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Paper-III: CH 103 (Physical Chemistry)

PC-01: Thermodynamics

PC-02: Electrochemistry

PC-03: Quantum Chemistry-I

PC-01: Thermodynamics

(15 hrs)

Third law of thermodynamics. Evaluation of absolute entropies from heat capacity data for solids, liquids and gases. Standard entropies.

Gibbs equations for non-equilibrium systems. Material equilibrium. Phase equilibrium. Clausius-Clapeyron equation. Conditions for equilibrium in a closed system. The chemical potential. Chemical potential of ideal gases. Ideal-gas reaction equilibrium-derivation of equilibrium constant. Temperature dependence of equilibrium constant-the van't Hoff equation.

Solutions: Partial molar properties-significance. Variation of chemical potential with T and P. Gibbs-Duhem equation-derivation and significance.

Ideal solutions. Thermodynamic properties of ideal solutions. Mixing quantities. Vapour pressure - Raoult's law. Thermodynamic properties of ideally dilute solutions. Vapour pressure- Henry's law.

Nonideal systems. Concept of fugacity, fugacity coefficient. Determination of fugacity. Non ideal solutions. Activities and activity coefficients. Standard-state conventions for non-ideal solutions.

Multicomponent phase equilibrium: Vapour pressure lowering, freezing point depression and boiling point elevation

PC-02: Electrochemistry

(15 hrs)

Electrochemical Cells: Derivation of Nernst equation – problems. Chemical and concentration cells (with and without transference). Liquid junction potential (LJP) – derivation of the expression for LJP – its determination and elimination.

Types of electrodes-Gas electrodes, Metal-metal ion electrodes, reference electrodes, indicator electrode, Ion selective electrodes, Metal-insoluble salt-anion electrodes, Redox electrodes.

Applications of EMF measurements: Solubility product, potentiometric titrations, determination of pH using glass electrode, equilibrium constant measurements. Decomposition potential and its significance. Electrode polarization – its causes and elimination. Concentration over-potential. Concept of activity and activity coefficients in electrolytic solutions. The mean ionic activity coefficient.

Debye-Huckel theory of electrolytic solutions: Debye-Huckel limiting law (derivation not required). Calculation of mean ionic activity coefficient. Limitations of Debye-Huckel theory. Extended Debye-Huckel's law. Theory of electrolytic conductance. Derivation of Debye-Huckel-Onsager equation – its validity and limitations.

PC-03: Quantum Chemistry- I

(15 hrs)

Wave mechanics and Schrödinger wave equation: Operators- Operator algebra. Commutation of operators, linear operators. Complex functions. Hermitian operators. Operators ∇ and ∇^2 . Eigenfunctions and eigenvalues. Degeneracy. Linear combination of eigenfunctions of an operator. Well behaved functions. Normalized and orthogonal functions.

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Postulates of quantum mechanics: Physical interpretation of wave function. Observables and Operators. Measurability of operators. Average values of observables. The time dependent Schrodinger equation. Separation of variables and the time-independent Schrodinger equation.

Theorems of quantum mechanics: Real nature of the eigen values of a Hermitian operatorsignificance. Orthogonal nature of the eigen values of a Hermitian operator-significance of orthogonality. Expansion of a function in terms of eigenvalues. Eigen functions of commuting operators-significance. Simultaneous measurement of properties and the uncertainty principle.

Particle in a box- one dimensional and three dimensional: Plots of ψ and ψ^2 -discussion. Degeneracy of energy levels. Calculations using wave functions of the particle in a box, orthogonality, measurability of energy, position and momentum, average values and probabilities. Application to the spectra of conjugated molecules.

References

1. Atkin's Physical Chemistry, Peter Atkins and Julio de Paula, Oxford University press
2. Physical Chemistry, Ira N. Levine, McGraw Hill
3. Physical Chemistry-A Molecular approach, D.A. McQuarrie and J.D. Simon, Viva Books Pvt. Ltd.
4. Molecular Thermodynamics, D.A. McQuarrie and J.D. Simon, University Science Books
5. Introduction to Electrochemistry, S. Glasstone; East-West Press (Pvt.) Ltd.
6. Modern Electrochemistry, J. O. M. Bockris & A. K. N. Reddy, Plenum
7. Principles of physical chemistry, Samuel H. Maron and Carl F. Prutton, Oxford & IBH
8. Physical Organic Chemistry, N. S. Isaacs, ELBS
09. Elementary Quantum Chemistry, F. L. Pilar, McGraw Hill.
10. Quantum Chemistry – D.A. McQuarrie, Viva Publication
11. Quantum Chemistry, Ira N. Levine, Prentice Hall
12. Introduction to Quantum Chemistry, A.K. Chandra, Tata McGraw Hill
13. Quantum Chemistry, R K Prasad, New Age International Pvt Ltd Publishers

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Paper-IV: CH 104 (Analytical Techniques and Spectroscopy – I)

ASP 01: Techniques of Chromatography & Electronic spectroscopy

ASP 02: NMR spectroscopy-I

ASP 03: Vibrational spectroscopy

ASP-01: Techniques of Chromatography and UV Visible Spectroscopy 15 hrs

Techniques of Chromatography: Introduction, Classification of chromatographic techniques, differential migration rates, partition ratio, retention time, relation between partition ratio and retention time, capacity factor, selectivity factor. Efficiency of separation - resolution, diffusion, plate theory and rate theory.

GC: Principle, instrumentation, detectors - TCD, FID, ECD. Derivatization techniques. Programmed temperature gas chromatography. GC analysis of hydrocarbons in a mixture.

HPLC: Principle, instrumentation, detectors- UV detectors, Photodiode array detector, fluorescence detector. HPLC analysis of paracetamol tablets.

UV Visible Spectroscopy: Principle, selection rules, Woodward-Fieser rules. Congugated dienes, trienes and polyenes. Unsaturated carbonyl compounds, Benzene, mono substituted derivative (Ph-R), di-substituted derivative (R-C₆H₄-R') and substituted benzene derivatives (R-C₆H₄-COR').

ASP 02: NMR spectroscopy-I 15 hrs

¹H NMR spectroscopy: Magnetic properties of nuclei, principles of NMR spectroscopy. Instrumentation: CW and pulsed FT instrumentation. Equivalent and non-equivalent protons. Homotopic, enantiotopic and diastereotopic protons. Chemical shifts, factors affecting the chemical shifts, electronegativity and anisotropy, shielding and deshielding effects. Signal integration. Spin-spin coupling, vicinal, germinal and long range coupling constants, factors affecting coupling constants. Chemically and magnetically equivalent protons.

Applications of ¹H NMR spectroscopy: Reaction mechanisms (cyclic bromonium ion, electrophilic and nucleophilic substitutions, carbocations and carbanions), E, Z isomers, conformation of cyclohexane and decalins, keto-enol tautomerism, hydrogen bonding, proton exchange processes (alcohols, amines and carboxylic acids), C-N rotation. Magnetic resonance imaging (MRI). ¹H-NMR of organic molecules and metal complexes: ethyl acetate, 2-butanone, mesitylene, paracetamol, aspirin, ethylbenzoate, benzyl acetate, 2-chloro propionic acid, [HNi(OPEt₃)₄]⁺, [HRh(CN)₅] (Rh I= 1/2).

ASP 03: Vibrational Spectroscopy 15 hrs

Interaction of electromagnetic radiation with matter. Factors affecting width and intensity of spectral lines.

IR Spectroscopy: Vibrational energy levels of diatomic molecules, selection rules (derivation not required). Calculation of force constant from vibrational frequency. Anharmonic oscillator. Morse potential energy diagram. Fundamental bands, overtones and hot bands, Fermi Resonance.

Vibration rotation spectra of diatomic and poly atomic molecules: Vibration - rotation spectroscopy, P, Q, R branches. Vibration - rotation spectra of polyatomic molecules - linear, symmetric top and asymmetric top molecules. Principles of FTIR.

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Vibrations of poly atomic molecules: Normal modes of vibration, concept of group frequencies. Characteristics of vibrational frequencies of functional groups; Stereochemical effects on the absorption pattern in carbonyl group, cis-trans isomerism and hydrogen bonding. Isotopic effect on group frequency.

Raman spectroscopy: Classical and quantum theories of Raman effect, Stokes and anti- Stokes lines. Complementary nature of IR and Raman spectra. Pure rotational, vibrational and vibrational – rotational Raman spectra. Selection rules. Depolarization factors of Raman lines and their relevance. Instrumentation and applications of Raman spectroscopy.

References

1. Fundamentals of Molecular Spectroscopy, Banwell and McCash McGraw Hill
2. Introduction to Molecular Spectroscopy, G.M. Barrow, McGrawHill
3. Absorption Spectroscopy of Organic Compounds, J.R. Dyer Prentice-Hall of India Pvt.Ltd
4. Introduction to Spectroscopy, Pavia Lampman Kriz. Cengage learning
5. Pharmaceutical analysis, Watson Elsevier
6. NMR in Chemistry- A multinuclear introduction, William Kemp, Springer
7. Organic Spectroscopy, William Kemp, Palgrave Macmillan
8. Spectroscopy of organic compounds, P.S. Kalsi, New Age International Publishers
9. Structural methods in Inorganic chemistry, E.A.V Ebsworth, John Wiley & Sons.
10. Organic Spectroscopy, LDS Yadav , Springer
11. Elementary Organic Spectroscopy, Y.R. Sharma S. Chand Limited
12. Molecular Spectroscopy by G Arhuldas, PHI Learning Private Ltd. New Delhi.
13. Vibrational Spectroscopy: Theory and Applications, D. N. Sathyanarayana, New Age International
14. Modern Spectroscopy, J. M. Hollas, John Wiley & Sons

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Practicals

Paper CH 151: Inorganic chemistry Lab course

4 hrs/week

I. Preparation of complexes

1. Hexaammine nickel (II) chloride.
2. Tris (acetylacetonato) manganese(III).
3. Tris(ethylenediamine) nickel(II) thiosulphate.

II. Calibrations

4. Calibration of weights.
5. Calibration of pipettes.
6. Calibration of standard flasks.
7. Calibration of burette.

III. Titrimetric Analysis

8. Estimation of Fe^{2+} by cerimetry
9. Estimation of Ni^{2+} by complexometry (direct titration method)
10. Estimation of Cu^{2+} by complexometry (direct titration method)
11. Estimation of Ca^{2+} by complexometry (substitution titration method)
12. Estimation of Ni^{2+} by complexometry (back titration method)
13. Estimation of Al^{3+} by complexometry (back titration method)

IV. One component Gravimetric Analysis

14. Estimation of Zn^{2+}
15. Estimation of Ba^{2+}

References

1. Text book of Quantitative Inorganic Analysis, 3rd edition, A.I.Vogel, ELBS (1969)
2. Vogel's text book of Quantitative Inorganic analysis, 4th edition, Jeffery etal, ELBS (1988).
3. Vogel's text book of Quantitative Inorganic Analysis, 6th edition, J.Mendham etal, Pearson education ltd (2002).
4. Practical Inorganic chemistry, G.Marr and B.W.Rockett, Van Nostrand Reinhold (1972).
5. Experimental Inorganic/Physical Chemistry – An Investigative integrated approach to Practical Project work, Mounir A.Malati, Woodhead publishing ltd (1999).
6. Advanced experimental Inorganic chemistry, Ayodhya Singh, Campus books international (2006)
7. Practical Inorganic Chemistry, G. Pass & H. Sutcliffe, University science books (1999)

Paper CH 152: Organic Chemistry Lab course

4 hours/ week

Synthesis of the following compounds:

- 1 p-Bromoacetanilide
- 2 p-Bromoaniline,
- 3 2,4,6- tribromoaniline

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- 4 1,3,5-Tribromobenzene
- 5 Tetrahydrocarbazole
- 6 7-Hydroxy-4-methyl coumarin
- 7 m-Dinitrobenzene
- 8 m-Nitroaniline
- 9 Hippuric acid
- 10 Azlactone
- 11 Anthracene-maleic anhydride adduct
- 12 2,4-Dihydroxyacetophenone
- 13 Phthalimide
- 14 Anthranilic acid
- 15 Methyl-4-nitrobenzoate

References

1. Text book of practical organic chemistry, Vogel
2. Text book of practical organic chemistry, Mann and Saunders.

Paper CH 153 Physical Chemistry Lab course

4 hrs / week

I. Data analysis I: Significant figures, Precision and accuracy

II. Chemical kinetics:

1. Acid-catalyzed hydrolysis of methyl acetate both with 1N HCl
2. Acid-catalyzed hydrolysis of methyl acetate both with 2N HCl
3. Peroxydisulphate-I⁻ reaction (overall order)
4. Oxidation of iodide ion by hydrogen peroxide-Iodine clock reaction.

III. Conductometry:

5. Determination of cell constant
6. Titration of strong acid vs strong base
7. Titration of weak acid vs strong base
8. Determination of dissociation constant of a weak acid

IV. Potentiometry:

9. Titration of strong acid vs strong base
10. Titration of weak acid vs strong base and determination of dissociation constant of a weak acid.
11. Determination of single electrode potential

V. Polarimetry:

12. Determination of specific rotation of sucrose
13. Determination of specific rotation of glucose
14. Determination of specific rotation of fructose

VI. Adsorption:

15. Adsorption of acetic acid on animal charcoal or silica gel

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References

1. Senior Practical Physical Chemistry B.D. Khosla, V.C. Garg and A. Khosla; R Chand & Co.
2. Experimental Physical Chemistry: V. Athawale and P. Mathur, New Age, International.
3. Practical Physical Chemistry: B. Vishwanathan and P.S. Raghavan, Viva Books.
4. Practical in Physical Chemistry: P.S. Sindhu, Laxmi Publications.
5. Advanced Practical Physical chemistry: J.B.Yadav, Krishna Prakashan Media

Paper CH 154: Analytical Chemistry -I Lab course

4 hrs/week

I. Applied analysis:

1. Estimation of acetic acid in commercial vinegar by acid base titration method
2. Estimation of iron in cement by dichrometry
3. Estimation of available chlorine in bleaching powder by iodometry
4. Estimation of calcium in calcium tablets by complexometry
5. Estimation of magnesium in talcum powder by complexometry

II. Thin layer chromatography

6. Determination of purity of the compounds prepared in CH 152]
7. Monitoring the progress of chemical reactions for any of the two preparations in CH 152

III. Assay of drugs:

8. Aspirin by acid base back-titration method
9. Ibuprofen by acid base titration method
10. Calcium in calcium gluconate by complexometry

IV. Determination of Physical Properties of Solutions:

11. Determination of molecular weight of a polymer by viscometry
12. Determination of critical solution temperature of phenol-water system
13. Effect of added electrolyte on the CST of phenol-water system

V. Colorimetry

14. Verification of Beer's law and calculation of molar extinction coefficient using CuSO_4 solution.
15. Verification of Beer's law and calculation of molar extinction coefficient using KMnO_4 solution

References

1. Advanced practical chemistry, R.Mukhopadhyay & P. Chatterjee, NCBA books (2016)
2. Advanced practical inorganic chemistry, Gurdeep Raj, GOEL publishing house (2015)
3. Advanced experimental Inorganic chemistry, Ayodhya Singh, Campus books Int. (2006)
4. Senior Practical Physical Chemistry: B.D. Khosla, V.C. Garg and A. Khosla
5. Advanced Practical Physical Chemistry: J.B.Yadav

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M.Sc. CHEMISTRY SYLLABUS
(Effective from academic year 2023-2024 for Campus, Constituent and Affiliated colleges)

SEMESTER –II

Semester-I and Semester-II syllabus is common for all specializations i.e., Inorganic, Organic, Physical, Physical- Organic, Analytical and Pharmacoinformatics.

Paper-I: CH 201 (Inorganic chemistry)

IC 04: Reaction mechanisms of transition metal complexes

IC 05: Bonding in metal complexes-II

IC 06: Metal clusters ligational aspects of diatomic molecules

IC-04: Reaction mechanisms of transition metal complexes: 15 hrs

Ligand substitution reactions: Energy profile of a reaction, transition state or activated complex. Types of substitution reactions: (SE, SN, SN¹, SN²). Langford-Gray classification: A mechanism, D-Mechanism, I-Mechanism I_a, I_d, and Intimate mechanism.

Ligand substitution reactions in octahedral complexes: Aquation or acid hydrolysis reactions, factors affecting acid hydrolysis. base Hydrolysis, conjugate base mechanism, evidences in favour of SN¹CB Mechanism. Substitution reactions without breaking metal-ligand bond. Anation reactions.

Ligand Substitution reactions in square-planar complexes: Mechanism of substitution in square-planar complexes, trans-effect, trans-influence, Grienberg's polarization theory and π - bonding theory, Applications of trans-effect in synthesis of Pt (II) complexes.

Electron transfer reactions (or oxidation-reduction reactions) in coordination compounds: Mechanism of one-electron transfer reactions, atom (or group) transfer or inner sphere mechanism, direct electron transfer or outer sphere mechanism, Factors affecting direct electron transfer reactions, Cross reactions and Marcus-Hush theory.

IC-05: Bonding in Metal Complexes – II: 15 hrs

Free ion terms and Energy levels: Configurations, terms, states and microstates. Calculation of the number of microstates for pⁿ and dⁿ configurations. Vector coupling of orbital angular momenta, spin angular momentum. Spin orbit coupling: L-S (Russel-Saunders) coupling scheme, j-j coupling scheme. Determination of terms for p¹, p², d¹ and d² configurations of metal ions. Hole formalism. Energy ordering of terms (Hund's rules). Inter – electron repulsion parameters (Racah parameters). Spin-orbital coupling parameters. Effect of weak cubic crystal fields on S, P, D and F terms. Orgel diagrams for (i) d¹, d⁴, d⁶, d⁹ (ii) d², d³, d⁷, d⁸ (iii) d⁵ octahedral and tetrahedral complexes.

IC-06: Metal Clusters and Ligational Aspects of Diatomic molecules 15 hrs

Metal Clusters: Definition, Factors favouring metal-metal bonding.

Metal carbonyl clusters: Bonding modes of CO: Terminal and bridging. 18 Valence electron rule and its applications. Classification of carbonyl clusters. Low nuclearity carbonyl clusters: M₃ and M₄ clusters, structural patterns in M₃(CO)₁₂ (M=Fe, Ru, Os) and M₄(CO)₁₂ (M=Co, Rh, Ir) clusters. High nuclearity carbonyl clusters: M₅, M₆, M₇, M₈ and M₁₀ clusters. Polyhedral skeletal electron pair theory

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and Total electron count theory. Capping rule. Structural patterns in $[\text{Ni}_5(\text{CO})_{12}]^{2-}$, $[\text{Os}_6(\text{CO})_{18}]^{2-}$, $[\text{Os}_7(\text{CO})_{21}]$, $[\text{Os}_8(\text{CO})_{22}]^{2-}$ and $[\text{Os}_{10}\text{C}(\text{CO})_{24}]^{2-}$. Metal carbonyl scrambling, stereo chemical non-rigidity in $[\text{Rh}_4(\text{CO})_{12}]$ and $[\text{Fe}_2(\text{Cp})_2(\text{CO})_4]$.

Boranes and carboranes: Wade's rules, STYX rule.

Metal Nitrosyls: Bonding modes of NO: Terminal (linear, bent) and bridging. Structural aspects of $[\text{IrCl}(\text{PPh}_3)_2(\text{CO})(\text{NO})]^+$ and $[\text{RuCl}(\text{PPh}_3)_2(\text{NO})_2]^+$. Stereo chemical control of valence in $[\text{Co}(\text{diars})_2(\text{NO})_2]^{2+}$ and $[\text{Co}(\text{diars})_2(\text{NO})(\text{SCN})]^+$.

Metal Halide clusters: Major structural types in dinuclear metal-metal systems: Edge sharing bioctahedra, face sharing bioctahedra, tetragonal prismatic and trigonal antiprismatic structures. Structure and bonding in $[\text{Re}_2\text{Cl}_8]^{2-}$ and octahedral halides of $[\text{Mo}_6(\text{Cl})_8]^{4+}$ and $[\text{Nb}_6(\text{Cl})_{12}]^{2+}$.

References

1. Inorganic reaction mechanisms, M.L.Tobe & John Burgess, Wesley Longman (1999)
2. Reaction mechanisms in metal complexes, K.Veera Reddy, New age publishers (2020)
3. Mechanisms of Reactions at Transition Metal Sites, Richard A Henderson, Oxford Science Primers, London (1993).
4. Mechanisms of inorganic reactions, F.Basalo & R.G.Pearson, 2nd Edition, John Wiley and sons, New York (1967)
5. Inorganic reaction mechanisms, R.K.Sharma, Discovery publishing house (2007)
6. Advanced Inorganic Chemistry. F.A.Cotton, G.Wilkinson, C.A.Murillo and M.Bochmann, 6th Edition, Wiley Interscience, N.Y (1999)
7. Principles of Inorganic Chemistry, Puri,Sharma, Kalia, 33rd Edition, Vishal Publications (2022).
8. Concise coordination chemistry, R Gopalan & V Ramalingam, Vikas publishing house Pvt Ltd (2008)
9. Selected topics in inorganic chemistry, Wahid U. Malik, G.D. Tuli & R.D. Madan, S.Chand & Co Ltd (1998)
10. Concise Inorganic Chemistry, J.D.Lee, 5th Edition, Chapman & Hall (2016).
Symmetry and Spectroscopy of Molecules. K.Veera Reddy, New Age International (P) Ltd. 2022.
11. Inorganic Chemistry, J.E. Huheey, K.A.Keiter and R.L.Keiter 4th Edition Harper Cottens College Publications (1993).
12. The Chemistry of Metal Cluster Complexes. D.F.Shriver, H.D.Kaerz and R.D.Adams (Eds), VCH, NY (1990).

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Paper-II: CH 202 (Organic Chemistry)

OC-04: Reaction mechanism-II and Molecular Rearrangements,

OC-05: Pericyclic reactions-I

OC-06: Photochemistry

OC-04: Reaction mechanism-II and Molecular Rearrangements

15 hrs

Neighbouring group participation (NGP) : Criteria for determining the participation of neighbouring group. Enhanced reaction rates, retention of configuration, isotopic labeling and cyclic intermediates. NGP involving Halogens, Oxygen, Sulphur, Nitrogen, Aryl. Introduction to nonclassical carbocations; NGP Cycloalkyl groups, σ and π - bonds. (Stereospecific examples of NGP to be covered in conformational analysis)

Reactive Intermediates: Generation, detection, structure, stability and reactions of carbenes and nitrenes.

Molecular rearrangements: Definition and classification. Molecular rearrangements involving 1) electron deficient carbon: Allylic and Wolf rearrangement. 2) electron deficient Nitrogen: Lossen, Curtius and Schmidt 3) electron deficient Oxygen: Baeyer-Villiger oxidation. 4) Base catalysed rearrangements: Benzilic acid, Favourski, Transannular, Sommelet-Hauser and Smiles rearrangement

OC-05 Pericyclic reactions

15 hrs.

Pericyclic reactions: Introduction, Classification of pericyclic reactions into Electrocyclic, cycloadditions, sigmatropic, ene and chelotropic reactions.

Electrocyclic reactions: con rotation and dis rotation. Electrocyclic closure and opening in $4n$ and $4n+2$ systems.

Cycloaddition reactions: Suprafacial and antara facial additions in $4n$ and $4n+2$ cycloadditions.

Sigmatropic reactions: [i, j] Suprafacial and antarafacial shifts, Cope and Claisen rearrangement reactions.

Approaches for the interpretation of mechanism of pericyclic reactions: Aromatic Transition States (ATS)/Perturbation Molecular Orbitals (PMO) approach-Concept of Huckel

-Möbius aromatic and antiaromatic transition states. Framing Woodward-Hofmann selection rules for all the pericyclic reactions by ATS approach. Solving problems based on ATS approach.

Molecular orbitals: ethylene, 1, 3-butadiene, 1, 3, 5-hexatriene, allyl cation, allyl radical, pentadienyl cation, pentadienyl radical.

Frontier Molecular Orbital (HOMO-LUMO) approach-concept: Framing Woodward-Hofmann selection rules for all the pericyclic reactions by Frontier Molecular Orbital (FMO) approach. Solving problems based on FMO approach.

Conservation of orbital symmetry: (Correlation Diagrams) approach- for electrocyclic and cycloadditions & cycloreversions.

OC-06 Organic Photochemistry

15hrs

Photochemistry: Introduction, photochemistry of π - π^* transitions: Excited states of alkenes, cis-trans isomerisation, and photo stationary state. Photochemistry of 1,3-butadiene, di- π methane

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rearrangement. Intermolecular reactions, photocycloadditions, photodimerisation of simple and conjugated olefins. Addition of olefins to α , β -unsaturated carbonyl compounds. Excited states of aromatic compounds, Photoisomerisation of benzene.

Photochemistry of ($n-\pi^*$) transitions: Excited states of carbonyl compounds, homolytic cleavage of α - bond, Norrish type I reactions in acyclic and cyclic ketones and strained cycloalkane diones. Intermolecular abstraction of hydrogen: photoreduction-influence of solvent, nature of hydrogen donor and structure of the substrate. Intramolecular abstraction of hydrogen: Norrish type II reactions in ketones, esters and 1,2-diketones, Addition to carbon-carbon multiple bonds, Paterno-Buchi reaction, Photochemistry of nitrites: Barton reaction.

References

1. Stereochemistry of Carbon compounds by Ernest L Eliel / Samuel H. Wilen
2. Stereochemistry of organic compounds – Principles and Applications by D Nasipuri
3. The third dimension in organic chemistry, by Alan Bassindale
4. Stereochemistry: Conformation and Mechanism by P S Kalsi
5. Stereochemistry by V M Potapov
6. Advanced Organic Chemistry by Jerry March
7. Mechanism and Structure in Organic Chemistry S. Mukerjee
8. Maya Shankar Singh, Reactive Intermediates in Organic Chemistry-Structure, mechanism and reactions, Wiley-VCH, 2012.
9. Organic chemistry Vol.I and II by I.L.Finar
10. Comprehensive organic chemistry Vol.5 D.H.R.Barton and W.D..Ollis
11. Pericyclic Reactions - A Textbook: Reactions, Applications and Theory by S. Sankararaman
12. Pericyclic reactions by Ian Fleming.
13. Organic photochemistry by J. M. Coxon and B, Halton
14. Introduction to organic Photochemistry by J. D. Coyle
15. Modern Molecular Photochemistry of Organic Molecules by N J Turro, V. Ramaswamy and J C Scaiano

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Paper-III: CH 203 (Physical Chemistry)

PC-04: Chemical Kinetics and Photochemistry

PC-05: Quantum Chemistry-II

PC-06: Solid State Chemistry:

PC-04: Chemical Kinetics & Photochemistry

(15 hrs)

Chemical Kinetics: Theories of reaction rates: Collision theory, steric factor. Transition state theory. Hammond's postulate. Thermodynamic formulation of transition state theory. Activation parameters and their significance. The Eyring equation. Unimolecular reactions and Lindemann's theory.

Complex reactions-Opposing reactions, parallel reactions and consecutive reactions (all first order type). Chain reactions-general characteristics, steady state treatment. Example- H_2-Br_2 reaction. Derivation of rate law.

Effect of structure on reactivity-Linear free energy relationships. Hammett and Taft equations-substituent (σ and σ^*) and reaction constant (ρ and ρ^*) with examples. Deviations from Hammett correlations, reasons- Change of mechanism, resonance interaction. Taft four parameter equation.

Photochemistry: The Franck Condon principle. Electronically excited molecules- singlet and triplet states. Radiative life times of excited states-theoretical treatment. Measured life times. Quantum yield. Derivation of fluorescence and phosphorescence quantum yields.

Photophysical processes- photophysical kinetics of unimolecular reactions. Calculation of rate constants of various photophysical processes-problems. Photosensitization. Quenching-Stern-Volmer equation. Introduction to fast reactions- Principle of flash photolysis.

PC-05: Quantum chemistry-II

(15 Hrs)

Cartesian, Polar and spherical polar coordinates and their interrelations. Schrodinger equation for the hydrogen atom- separation into three equations. Hydrogen like wave functions. Radial and angular functions. Quantum numbers n , l and m and their importance. The radial distribution functions. Hydrogen like orbitals and their representation. Polar plots, contour plots and boundary diagrams.

Many electron systems: Approximate methods. The variation method-variation theorem and its proof. Trial variation function and variation integral. Examples of variational calculations. Particle in a box. Construction of trial function by the method of linear combinations. Variation parameters. Secular equations and secular determinant.

Bonding in molecules: Molecular orbital theory-basic ideas. Construction of MOs by LCAO, H_2^+ ion. The variation integral for H_2^+ ion. Detailed calculation of wave functions and energies for the bonding and antibonding MOs. Physical picture of bonding and antibonding wave functions, energy diagram. The MO wave function and the energy of H_2 molecule MO by LCAO method and Valence bond method (detailed calculations not required)-comparison of MO and VB models.

PC-06: Solid state chemistry

(15 Hrs)

Electronic properties of metals, insulators and semi-conductors: Electronic structure of solids, Band theory, Fermi level, K space and Brillouin Zones, band structure of metals, insulators and semi-conductors. Electrons, holes and Excitons. The temperature dependence of conductivity of extrinsic semi-conductors. Photo conductivity and photovoltaic effect - p-n junctions.

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Superconductivity: Occurrence of superconductivity. Destruction of superconductivity by magnetic fields – Meissner effect. Types of superconductors. Theories of super conductivity – BCS theory. High temperature superconductors: Structure of defect perovskites. High T_c superconductivity in cuprates. Phase diagram of Y-Ba-Cu-O system. Crystal structure of $YBa_2Cu_3O_{7-x}$. Preparation of 1-2-3 materials. Origin of high T_c superconductivity.

Nanoparticles and their applications: Introduction to nanoparticles. Reduced dimensionality in solids: systems with various dimensions -examples.

Preparation of nano particles – top down and bottom up methods. Preparation of nanomaterials- – sol gel methods, chemical vapour deposition method and thermolysis. Characterization of nanoparticles – experimental methods – Powder X-ray Diffraction, Scanning electron microscope (SEM), Transmission Electron Microscopy (TEM), and Atomic Force Microscopy (AFM) (Instrumentation not required). Optical properties of nanoparticles. Applications of nanoparticles.

References

1. Physical Chemistry-A Molecular approach, D.A. McQuarrie and J.D. Simon, Viva Books Pvt Ltd
2. Elements of Physical Chemistry by Peter Atkins and Julio de Paula, Oxford University Press
3. Chemical Kinetics and Reaction Mechanisms, J. H. Espenson, McGraw Hill
4. Chemical Kinetics, K.J. Laidler, McGraw Hill
5. The Physical Basis of Org. Chemistry by Howard Maskill, Oxford Univ. Press (New York)
6. Fundamentals of Photochemistry, K.K.Rohtagi-Mukherji, Wiley-Eastern
7. Molecular Reactions and Photo chemistry by Depuy and Chapman
8. Molecular Photochemistry, N.J. Turro, Benjamin
9. Photochemistry, R.P.Kundall and A. Gilbert, Thomson Nelson
10. Essentials of Molecular Photochemistry by A. Gilbert and J. Baggott, Blackwell Scientific Publications.
11. Organic Photochemistry by J.M.Coxon and B.Halton, Cambridge University press.
12. Introductory Photochemistry by A.Cox and T.J.Kemp. McGraw-Hill, London.
13. Quantum Chemistry, D.A. McQuarrie, Prentice Hall
14. Quantum Chemistry, Ira N. Levine, Prentice Hall
15. Introduction to Quantum Chemistry, A.K. Chandra, Tata McGraw Hill
16. Quantum Chemistry, R K Prasad, New Age International Pvt Ltd Publishers
17. Elementary Quantum Chemistry, F. L. Pilar, McGraw Hill.
18. Introduction to Solids, Leonid V. Azaroff, Tata McGraw Hill
19. Solid state Chemistry, D.K. Chakrabarthy, New Age International
20. Solid state Chemistry and its applications, A.R. West, Plenum.
21. Principles of the Solid State, H. V. Keer, New Age International
22. The physics and chemistry of solids by Stephen Elliott, Wiley Publishers.
23. Nanostructured Materials and Nanotechnology, edited by Hari Singh Nalwa, Acad. Press
24. Self-Assembled Nanostructures, Jin Zhang, Zhong-lin Wang, Jun Liu, Shaowei Chen & Gan-Yu-Liu, Kluwer Academic/Plenum
25. Introduction to Nanotechnology, Charles P. Poole Jr, F. J. Owens, Wiley India Pvt. Ltd.

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Paper-IV: CH 204 (Analytical Techniques and Spectroscopy – II)

15 hrs

ASP 04: Electro and Thermal Analytical Techniques

ASP 05: NMR-II and ESR Spectroscopy

ASP 06: Mass spectrometry

ASP- 04: Electro and Thermal Analytical Techniques

Electro analytical techniques: Types and Classification of Electro analytical Methods.

Polarography: Types of polarography: A.C Polarography and D.C Polarography. D.C Polarography: Instrumentation - Dropping mercury electrode, polarogram. Types of Currents: Residual, Migration and Limiting currents. Two and Three electrode assemblies. Ilkovic equation (derivation not necessary) and its consequences. Applications of polarography in qualitative and quantitative analysis. Analysis of mixtures. Application to inorganic and organic compounds. Determination of stability constants of complexes.

Amperometric titrations: Principle, Instrumentation. Types and applications of amperometric titrations. Determination of SO_4^{2-} , metal ions viz., Mg^{2+} , Zn^{2+} , Cu^{2+} and other substances.

Cyclic Voltammetry: Principle, instrumentation, Applications. Cyclic voltammetric study of insecticide parathion. HOMO-LUMO calculations of ferrocene using cyclic voltammetry.

Thermal Analysis:

Introduction, types of thermo analytical methods.

Thermogravimetry: Principle and applications of thermogravimetry- Study of calcium oxalate, calcium sulphate and silver nitrate, Differential thermal analysis: Principle and applications of DTA- Differential thermogram of sulphur,

Differential scanning calorimetry DSC: Principle and application of DSC- determination of glass transition temperatures and heat capacities of PVC and Bakelite.

ASP- 05: NMR-II and ESR Spectroscopy

15 hrs

Multinuclear NMR (^1H , ^{19}F and ^{31}P NMR) and solid state NMR spectroscopy:

First order and non-first order spectra e.g., AX, AX₂, AX₃, A₂X₃, AMX and AB, ABC. Simplification of complex spectra: increased field strength, deuterium exchange, Lanthanide shift reagents and double resonance techniques. Discrimination of enantiomers by use of chiral NMR solvents (CSAs), chiral lanthanide shift reagents and Mosher's acid. Nuclear Overhauser Enhancement (NOE). Fluxional molecules bullvalene, $[\eta^1\text{-C}_5\text{H}_5\text{M}]$, $[\eta^5\text{-(C}_5\text{H}_5)_2\text{Ti}\eta^1\text{-(C}_5\text{H}_5)_2]$ and $[\eta^4\text{-C}_8\text{H}_8\text{Ru(CO)}_3]$.

^{19}F NMR spectroscopy: ^{19}F chemical shifts, coupling constants. Applications of ^{19}F NMR involving coupling with ^{19}F , ^1H and ^{31}P : 1,2-dichloro-1,1-difluoro ethane, BrF_5 , SF_4 , PF_5 , ClF_3 , IF_5 , $\text{CF}_3\text{CH}_2\text{OH}$.

^{31}P NMR spectroscopy: ^{31}P chemical shifts, coupling constants. Applications of ^{31}P NMR involving coupling with ^{31}P , ^{19}F , ^1H and ^{13}C : ATP, Ph_3PSe , P_4S_3 , H_3PO_4 , H_3PO_3 , H_3PO_2 , HPF_2 , PF_6^- , PH_3 , $[\text{Rh}(\text{PPh}_3)_3\text{Cl}]$ (Rh: I= 1/2).

Introduction to solid state NMR: Magic angle spinning (MAS). Applications of solid state NMR.

Electron Spin Resonance Spectroscopy: Introduction, principle, instrumentation, selection rules, calculation of 'g'. Study of free radicals.

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ASP - 06: Mass spectrometry

15 hrs

Origin of mass spectrum, principle of EI mass spectrometer. Types of fragments: Odd electron and even electron containing neutral and charged species (even electron rule), Nitrogen rule, isotopic peaks, determination of molecular formula, metastable ion peaks. High resolution mass spectrometry. Salient features of fragmentation pattern of organic compounds including β -cleavage, McLafferty rearrangement, retro Diels – Alder fragmentation and ortho effect.

Principle of EI, CI, Atmospheric Pressure Ionisation (API), Secondary Ion Mass Spectrometry (SIMS), Electrospray ionization (ESI) and Matrix Assisted Laser Desorption Ionization (MALDI) methods.

Introduction, principle and applications of Gas Chromatography-Mass Spectrometry (GC-MS) and Liquid chromatography-Mass Spectrometry (LC-MS) techniques.

References:

1. Principles of Polarography, Heyrovsky, Elsevier Inc.
2. Principles of Polarography, Kapoor, John Wiley & Sons.
3. Modern Electroanalytical methods, edited by C.C harlot, Elsevier Company.
4. Principles of Instrumental analysis, Skoog, Holler and Nieman, Harcourt Asia PTE Ltd.
5. Analytical Chemistry-An Introduction, Skoog, West, Holler and Crouch, Saunders College Publishing.
6. Principles of Instrumental Analysis, Skoog and Leary, Saunders College Publishing.
7. Spectroscopic identification of organic compounds by R.M. Silverstein and F.X. Webster, John Wiley & Sons
8. Instrumental Methods of Chemical Analysis by B K Sharma, Krishna Prakashan Pvt. Ltd.
9. Instrumental Methods of Analysis by Willard, New York, Van Nostrand
10. Organic spectroscopy by William Kemp, Palgrave Macmillan.
11. NMR-A multinuclear introduction by William Kemp, Springer
12. Spectroscopic methods in organic chemistry by D.H. Williams and I. Fleming McGraw-Hill Education

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Practicals

Paper CH 251: Inorganic chemistry Lab course

4 hours/ week

I. Preparation of complexes:

1. Mercury tetrathiocyanatocobaltate(II).
2. Chloropentamminecobalt(III) chloride
3. Tetramminecopper(II) sulphate

II. Titrimetric Analysis of two ions in a mixture

4. Estimation of Pb^{2+} and Ca^{2+}
5. Estimation of Zn^{2+} and Mg^{2+}
6. Estimation of Mg^{2+} and Mn^{2+}

III. Analysis of Two component mixtures

- 7, 8. Separation of Ag^+ and Ca^{2+} in a mixture and estimation of Ag^{2+} (gravimetric) and Ca^{2+} (volumetric).
- 9, 10. Separation of Cu^{2+} and Ni^{2+} in a mixture and estimation of Ni^{2+} (gravimetric) and Cu^{2+} (volumetric)
- 11, 12. Separation of Fe^{3+} and Al^{3+} in a mixture and estimation of Fe^{3+} (volumetric) and Al^{3+} (gravimetric).

IV. Analysis of three component mixtures:

13. Separation of (Ni^{2+} and Cu^{2+}) from Mg^{2+} in the given mixture and estimation of Mg^{2+} gravimetrically

V. Ion exchange methods of analysis:

14. Determination of capacity of an ion exchange resin.
15. Separation of Mg^{2+} and Zn^{2+} on an anion exchange resin and estimation of Mg^{2+} and Zn^{2+}

References

1. Text book of Quantitative Inorganic Analysis, 3rd edition, A.I.Vogel, ELBS (1969)
2. Vogel's text book of Quantitative Inorganic analysis, 4th edition, Jeffery etal, ELBS (1988).
3. Vogel's text book of Quantitative Inorganic Analysis, 6th edition, J.Mendham etal, Pearson education ltd (2002).
4. Practical Inorganic chemistry, G.Marr and B.W.Rockett, Van Nostrand Reinhold (1972).
5. Experimental Inorganic/Physical Chemistry – An Investigative integrated approach to Practical Project work, Mounir A.Malati, Woodhead publishing ltd (1999).
6. Advanced experimental Inorganic chemistry, Ayodhya Singh, Campus books international (2006)
7. Practical Inorganic Chemistry, G. Pass & H. Sutcliffe, University science books (1999)

Paper CH 252: Organic Chemistry Lab course

4 hours/ week

Identification of organic compounds systematic qualitative analysis:

1. BP / MP, Ignition test, solubility classification
2. Extra elements-N,S & Halogens,(Lassaigne sodium fusion test)
3. p-Nitrobenzoic acid/2-Chloro benzoic Acid

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4. Anisole
5. p- Chlorophenol
6. p-Chloroanilines
7. N-Methyl aniline/N-Ethylaniline
8. N,N-Dimethylaniline
9. Benzamide
10. p-Chloro benzaldehyde
11. Acetophenone/ P-Chloro acetophenone,
12. Benzophenone
13. Nitrobenzene
14. Ethylbenzoate
15. Chlorobenzene/ Bromobenzene

References

1. Text book of practical organic chemistry, Vogel
2. Text book of practical organic chemistry, Mann and Saunders.
3. Spectral identification of organic compounds Bassler, Silverstein 5th Edition

Paper CH 253: Physical Chemistry Lab

4hrs /week

I. **Data analysis II:** Mean and standard deviation; absolute and relative errors; linear regression; covariance and correlation coefficient.

II. Distribution:

1. Distribution of I₂ between cyclohexane and water
2. Distribution of I₂ between cyclohexane and aq. KI solution - calculation of equilibrium constant.

III. Chemical Kinetics:

3. Stoichiometry of Peroxydisulphate - Iodide reaction
- 4,5. Peroxydisulphate - Iodide reaction: Comparison of strengths of KI solutions by isolation method

IV. Conductometry:

6. Titration of a mixture of strong and weak acids vs strong base
7. Determination of the hydrolysis constant of aniline hydrochloride
8. Determination of solubility product

V. Potentiometry:

9. Titration of Cl⁻ vs Ag⁺ (precipitation titration)
10. Determination of solubility product of sparingly soluble salt

VI. Polarimetry:

11. Inversion of cane sugar catalyzed by 1N HCl
12. Inversion of cane sugar catalyzed by 2N HCl

V. pH metry:

13. Calibration of a pH meter and preparation of phosphate buffers
14. Titration of strong acid vs strong base
15. Titration of weak acid vs strong base and determination of dissociation constant of weak acid

References

1. Senior Practical Physical Chemistry B.D. Khosla, V.C. Garg and A. Khosla; R Chand & Co.
2. Experimental Physical Chemistry: V. Athawale and P. Mathur, New Age, International.
3. Practical Physical Chemistry: B. Vishwanathan and P.S. Raghavan, Viva Books.
4. Practical in Physical Chemistry: P.S. Sindhu, Laxmi Publications.
5. Advanced Practical Physical chemistry: J.B.Yadav, Krishna Prakashan Media

Paper CH 254: Analytical Chemistry -II & Spectroscopy Lab course

4 hours/ week

I. Applied analysis:

1. Estimation of alkali content in antacid by acid base titration method
2. Estimation of ascorbic acid in vitamin C by iodometry
3. Estimation of available oxygen in hydrogen peroxide by permanganometry
4. Estimation of calcium in milk by complexometry
5. Determination of hardness of water by complexometry.

II. Spectral analysis: Interpretation of IR, UV, ^1H NMR and MS of the following representative compounds

6. An aldehyde
7. An alcohol
8. A carboxylic acid
9. An amine
10. A Ketone

III. Instrumental Analysis:

Conductometry:

11. Titration of a mixture of strong and weak acids vs weak base

Potentiometry:

12. Titration of Fe^{+2} vs $\text{Cr}_2\text{O}_7^{2-}$ (redox titration)
13. Fe^{2+} vs Ce^{4+} and calculation of formal redox potential of Fe(II)/Fe(III)
14. Fe^{2+} vs MnO_4^- and calculation of formal redox potential of Fe(II)/Fe(III)

pH metry:

15. Titration of a mixture of strong and weak acids vs strong base

References:

1. Vogel's text book of Quantitative Inorganic Analysis, 6th edition, J.Mendham etal, Pearson education ltd (2002)
2. Advanced practical chemistry, R.Mukhopadhyay & P. Chatterjee, NCBA books (2016)
3. Advanced practical inorganic chemistry, Gurdeep Raj, GOEL publishing house (2015)
4. Advanced experimental Inorganic chemistry, Ayodhya Singh, Campus Books International (2006)
5. Senior Practical Physical Chemistry: B.D. Khosla, V.C. Garg and A. Khosla
6. Advanced Practical Physical Chemistry: J.B.Yadav
7. Organic structures from spectra: L. D. Field, S. Sternhell, J. R. Kalman.

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M.Sc. CHEMISTRY

**PHYSICAL CHEMISTRY SPECIALISATION
SYLLABUS OF III & IV SEMESTERS
*REVISED AS PER NEW (CB) SYLLABUS***

**FOR STUDENTS ADMITTED FROM THE YEAR
2016 ONWARDS**

M.Sc. CHEMISTRY (PHYSICAL CHEMISTRY SPECIALISATION)

Syllabus for III and IV Semesters

(for the batches admitted in academic year 2016 & later under CBCS pattern)

[Under Restructured CBCS Scheme]

Grand total marks and credits (all 4 semesters) 2400 marks – 96 credits

(Approved in the P.G. BOS meeting held on 01-07-2017)

Semester - III (Physical Chemistry)

[Under CBCS Scheme]

(for the batches admitted in academic year 2016 & later under CBCS pattern)

	Hrs/week	Internal assessment	Semester exam	Total	Credits
CH(PC)301T (core)	4	20 marks	80 marks	100 marks	4
CH(PC)302T (core)	4	20 marks	80 marks	100 marks	4
CH(PC)303T (Elective)	4	20 marks	80 marks	100 marks	4
CH(PC)304T (Elective)	4	20 marks	80 marks	100 marks	4
CH(PC)351P (LAB-I)	9			100 marks	4
CH(PC)352P (LAB-II)	9			100 marks	4
Total				600 marks	24

Semester - IV (Physical Chemistry)

	Hrs/week	Internal assessment	Semester exam	Total	Credits
CH(PC)401T (core)	4	20 marks	80 marks	100 marks	4
CH(PC)402T (core)	4	20 marks	80 marks	100 marks	4
CH(PC)403T (Elective)	4	20 marks	80 marks	100 marks	4
CH(PC)404T (Elective)	4	20 marks	80 marks	100 marks	4
CH(PC)451P (LAB-I)	9			100 marks	4
CH(PC)452P (LAB-II)	9			100 marks	4
Total				600 marks	24

Grand total marks and credits (all 4 semesters) 2400 marks - 96 credits

M.Sc. SEMESTER - III
PHYSICAL CHEMISTRY SPECIALIZATION
(for the batches admitted in academic year 2016 & later under CBCS pattern)

PAPER –CH(PC) 301T: QUANTUM CHEMISTRY AND GROUP THEORY

- PC - 09: Applications of Schrödinger equation
- PC - 10: Angular momentum & approximate methods
- PC - 11: Bonding in molecules
- PC - 12: Group theory

PAPER – II CH (PC) 302T : SPECTROSCOPY AND LASERS

- PC- 13 : Physical principles of spectroscopy and Vibrational spectroscopy
- PC- 14 : NMR , NQR and Mossbauer Spectroscopy
- PC- 15 : X-ray Spectroscopy & Diffraction techniques
- PC- 16 : Lasers in Chemistry

ELECTIVE 3A

PAPER III CH (PC) 303T(CB1) : APPLIED CHEMISTRY, MATERIAL SCIENCE AND RADIATION EFFECTS

- PC(CB1)-1 : Applied kinetics
- PC(CB1)-2 : Applied Electrochemistry
- PC(CB1)-3 : Types of materials, conducting organics and NLO materials
- PC(CB1)-4 : Radiation effects

ELECTIVE–3B

Paper-III CH (PC) 303T(CB2): Biopolymer Chemistry

- PC-(CB2)- 5: Bioenergetics and physical properties of biopolymers
- PC-(CB2)- 6: Biological membranes and binding of ligands by biopolymers
- PC-(CB2) - 7: DNA, genes and cloning
- PC-(CB2) - 8: Bioinformatics

ELECTIVE–4A

PAPER-IV CH(PC) 304T(CB3): Polymer Chemistry

- PC-(CB3)-9: Polymerization and Kinetics of polymerization
- PC-(CB3)-10: Structure and properties of polymers
- PC-(CB3)-11: Processing of Polymers
- PC-(CB3)-12: Functional polymers

ELECTIVE –4B

Paper IV CH(PC) 304T(CB4): Environmental Chemistry

- PC(CB4)-13: Pollution in Atmosphere
- PC(CB4)-14: Pollution in Hydrosphere
- PC(CB4)-15: Heavy Metal and Radiochemical Pollution.
- PC(CB4)-16: Analysis of Air, Water and Metal Pollutants

LABORATORY COURSES

Paper-V CH (PC) 351 P: Chemical Kinetics

Paper-VI CH(PC) 352P: Instrumentation

**M.Sc. SEMESTER - IV
PHYSICAL CHEMISTRY SPECIALIZATION**

(for the batches admitted in the academic year 2016 and later under CBCS pattern)

PAPER-1 CH(PC) 401T(CB1): Thermodynamics, Chemical Kinetics and Electrochemistry

- PC- 17. Statistical Thermodynamics
- PC- 18. Non-equilibrium Thermodynamics
- PC- 19. Chemical Kinetics-II
- PC- 20. Electrochemistry –II

PAPER-II CH(PC) 402T: Supramolecular chemistry, Photo Chemistry and Computational chemistry

- PC-21 : Supramolecular Chemistry
- PC-22 : Photochemistry-II
- PC-23 : Computational Chemistry
- PC-24: Theoretical treatment of bio polymers

ELECTIVE–3A

PAPER-III CH(PC) 403 T(CB1) : Catalysis

- PC-(CB1)-17: Homogeneous catalysis
- PC-(CB1)-18: Surface Chemistry and Micellar catalysis
- PC-(CB1)-19: Heterogeneous catalysis
- PC-(CB1)-20: Phase transfer , Anchored and Photo catalysis

ELECTIVE–3B

Paper IV CH(PC) 403 T(CB2) : Dynamics of chemical reactions and Sensors

- PC-(CB2)-21: MO and VB theory of reactivity
- PC-(CB2)-22: Kinetic, isotopic, structural, solvent, steric and conformational effects
- PC-(CB2)-23: Nucleophilic, electrophilic and free radical reactivity
- PC-(CB2)-24: Sensors

ELECTIVE –4A (ID PAPER)

PAPER-IV CH(PC) – 404T(CB3) : Computational Chemistry and It's Applications

- PC(CB3)-25: Computational Chemistry – I
- PC(CB3)-26: Computational Chemistry – II
- PC(CB3)-27: Drug Design Methods I - Ligand Based
- PC(CB3)-28: Drug Design Methods II - Structure Based.

ELECTIVE–4B (ID PAPER)

PAPER-IV CH(PC) 404T(CB4): Engineering Chemistry

- PC(CB4) -29: Water And Waste Water Treatment
- PC(CB4) -30: Corrosion And Its Control
- PC(CB4) -31: Energy Sources:
- PC(CB4)- 32 Engineering Materials.

ELECTIVE–4C (ID PAPER)

PAPER-IV CH(PC) 405T(CB5): Sugar Chemistry and Sugar Technology

- PC(CB5) -33: Advanced Sugar Chemistry
- PC(CB5) -34: Sugar and Sugar byproducts
- PC(CB5) -35: Methodology used in Sugar Analysis
- PC(CB5)- 36: Sugar Technology and Management

LABORATORY COURSES

- Paper-V CH (PC) 451P: Chemical Kinetics
- Paper-VI CH (PC) 452P: Instrumentation

M.Sc. SEMESTER - III
PHYSICAL CHEMISTRY Specialization
 (for the batches admitted in academic year 2016 and later under CBCS pattern)

PAPER –CH(PC) 301T: QUANTUM CHEMISTRY AND GROUP THEORY

PC -09: Applications of Schrödinger equation
 PC -10: Angular momentum and approximate methods
 PC -11: Bonding in molecules
 PC -12: Group theory

PC-09: Applications of Schrödinger equation (15 hrs)

Systems with discontinuity in the potential field. A simple potential barrier. A potential barrier with a finite thickness. Quantum mechanical tunneling – examples - α -particle emission, inversion of NH_3 , hydrogen transfer reactions.

The harmonic oscillator – detailed treatment. Wave functions and energies. Vibration of a diatomic molecule – harmonic oscillator model.

The rigid rotator – detailed treatment. Wave functions and energies. Spherical harmonics. Rigid rotator as model for a rotating diatomic molecule.

The hydrogen atom – detailed treatment. Angular and radial functions. Atomic orbitals. Measurability of the ground-state energy of hydrogen atom. Orthonormal nature of hydrogen-like wave functions. Probability calculations.

Atomic and molecular term symbols.

Atoms in external field, Zeeman and anomalous Zeeman effect.

PC-10: Angular momentum and approximate methods (15 hrs)

Angular momentum operators. Commutation relations of angular momentum operators and their consequence. Eigen functions of L^2 and L_z and the eigen values. Magnitude and orientation of angular momentum vectors.

Electron spin. Spin operators. Pauli principle and the Pauli exclusion principle.

Approximate methods- The variation method. Construction of variation function by the method of linear combinations. H and He atom. Perturbation theory (first order and nondegenerate). Wave function and energy corrections. Application of perturbation theory to the helium atom.

Time- dependent perturbation theory. Interaction of radiation and matter. Allowed and forbidden transitions.

Multielectron atoms. The Hartree-Fock self-consistent field method. Basis functions. Slater-type orbitals (STOs).

PC-11: Bonding in molecules

(15 hrs)

Born-Oppenheimer approximation. MO theory of H_2^+ ion. Calculation of MOs and their energies. Evaluation of the overlap integral. Probability curves and energy diagram. MO theory of H_2 molecule. Calculation of energy. MO theory of polyatomic molecules (general ideas). MO treatment of H_2O . Symmetry-adapted linear combinations. MOs of H_2O .

Concept of hybridization – sp, sp^2 , and sp^3 hybrid orbitals.

Semiempirical MO methods. The Hückel theory of conjugated systems. HMO calculations on ethylene, allyl system, butadiene, cyclopropenyl system and benzene. π -electron charges and bond orders. Simplification of secular determinants of cyclopropenyl system, cyclobutadiene and benzene using molecular symmetry. Introduction to extended Hückel Theory, extension of the Hückel's approach to molecules containing heteroatoms.

Orbital symmetry and reactivity: $\text{H}_2 + \text{F}_2 \rightarrow 2\text{HF}$ reaction. $2\text{NO} \rightarrow \text{N}_2 + \text{O}_2$ reaction.

PC-12: Group theory

(15 hrs)

Matrices: Addition and multiplication of matrices. Diagonal matrix. Unit matrix. Transpose of a matrix. Adjoint of a matrix. Inverse of a matrix. The determinant of a square matrix. Expansion of a determinant. Properties of determinants.

Symmetry operations forming a group. Classes of symmetry operations. Matrix representation of symmetry operations and point groups. Generation of representations for point groups. Reducible and irreducible representations.

The Great Orthogonality theorem (proof not required) and its consequences. Relation between reducible and irreducible representations. Character tables. Construction of character tables for C_{2h} , C_{2v} and C_{3v} groups.

Quantum mechanics and group theory. Wave functions as bases for irreducible representations. The direct product – vanishing of integrals. Projection operators. Symmetries of vibrations. IR and Raman activity.

Books suggested:

1. Quantum Chemistry, Ira N. Levine, Prentice Hall
2. Introduction to Quantum Chemistry, A. K. Chandra, Tata McGraw Hill
3. Elementary Quantum Chemistry, F. L. Pilar, McGraw Hill
4. Molecular Quantum Mechanics, P. W. Atkins & R. S. Friedman, Oxford University Press
5. Coulson's Valence, R. McWeeny, ELBS
6. The Chemical Bond, J. N. Murrell, S. F. A. Kettle & J. M. Tedder, John Wiley
7. Valency Theory, J. N. Murrell, S. F. A. Kettle & J. M. Tedder, ELBS
8. Chemical Applications of Group Theory, F. A. Cotton, John Wiley & Sons
9. Symmetry and Group Theory In Chemistry, Mark Ladd, Harwood Publishers, London (2000).
10. Symmetry Through the Eyes of a Chemist, I. Hargittai and M. Hargittai, 2nd Edition, Plenum Press, NY (1995).
11. Molecular Symmetry and Group Theory, Robert L. Carter, John Wiley & Sons (1998).
12. Group Theory for Chemists, G. Davidson, Macmillan Physical Science Series (1991).

PAPER – II CH (PC) 302T : SPECTROSCOPY AND LASERS

PC- 13 : Physical principles of spectroscopy and Vibrational spectroscopy

PC- 14 : NMR , NQR and Mossbauer Spectroscopy

PC- 15 : X-ray Spectroscopy and Diffraction techniques

PC- 16 : lasers in Chemistry

PC-13: Physical principles of spectroscopy and Vibrational spectroscopy:

(15 Hrs)

Interaction of electromagnetic radiation with matter. Absorption and emission of radiation. Induced absorption, spontaneous emission and stimulated emission. Oscillator strength, transition moment integral. Selection rules, Spectrum of formaldehyde. Factors affecting width and intensity of spectral lines -Line width and natural line broadening, doppler broadening. Intensity of spectral lines.

Infrared spectroscopy- Anharmonic oscillator. Morse potential energy diagram.

Vibration – rotation spectroscopy, P, Q, R branches. Vibration – rotation spectra of polyatomic molecules – linear, symmetric top and asymmetric top molecules. Principles of FTIR.

Raman spectroscopy- Classical and quantum theories of Raman effect. Pure rotational, vibrational and vibrational – rotational Raman spectra. Selection rules. Depolarization factors of Raman lines and their relevance. Instrumentation. Typical applications of Raman spectroscopy – Structure determination of XY_4 molecules, Phase transitions.

PC-14: NMR, NQR and Mossbauer Spectroscopy.

(15hrs)

Principle of nmr. Derivation of $h \nu = g \beta H$. Larmor precessional frequency- spin-spin splitting (AX) - Quantitative treatment (proof for J= distance between two successive nmr spectral lines) – Instrumentation - CW instrument and FT instrument.

Two dimensional nmr spectroscopy:

Principles of 2D nmr-Graphical representation of 2D nmr spectra – Homonuclear 1H J, δ spectroscopy-its application for mixture analysis- (for instance mixture analysis of n-butyl bromide and n-butyl iodide) - The COSY experiment. Two dimensional 1H , 1H shift correlations. COSY spectra of an AX system, o-nitroaniline, alanine, glutamic acid and arginine.

The nuclear overhauser effect(NOE). wo dimensional nuclear overhauser spectroscopy(NOESY). Nuclear Quadrupole Resonance: Quadrupole nuclei and quadrupole moments-prolate and oblate nuclear charge distributions-energies of quadrupolar transitions-electric field gradient, coupling constants and splitting.

Mossbauer Spectroscopy - Mossbauer effect – Recoil energy, typical Mossbauer spectrum - isomer shift – quadrupole splitting – magnetic hyperfine interaction – ^{57}Fe – Mossbauer spectra of Fe^{2+} and Fe^{3+} (paramagnetic) and Fe^{3+} (magnetic) compounds.

PC-15: X-ray Spectroscopy and Diffraction techniques:

(15 hrs)

X-ray fluorescence (XRF) : Experimental method, Processes in X-ray fluorescence, K-emission spectrum of tin, L-emission spectrum of gold.

X-ray absorption: Absorption techniques, Absorption edge fine structure (AEFS spectra) and extended X-ray absorption fine structure (EXAFS) spectra.

X-ray diffraction: Bragg condition. Miller indices, d-spacing formula, Lattice planes and number of d-spacings, experimental methods of X-ray diffraction. Laue method and Debye-Scherrer method. Primitive and nonprimitive unit cells. Indexing the reflections. Identification of unit cells from systematic absences in diffraction pattern. Structure factor and its relation to intensity and electron density. Description of the procedure for an X-ray structure analysis. Typical examples.

Electron diffraction. Scattering intensity versus scattering angle. Wierl equation. Measurement technique. Elucidation of structure of simple gas phase molecules.

PC-16: Lasers in Chemistry:

(15 hrs)

General principles of laser action. Stimulated emission. Rates of absorption and emission. Population inversion. Three-level and four-level laser systems. Pumping. Laser cavity – resonant modes. Characteristics of laser light. Laser pulses and their characteristics. Pulse production, Q-switching. Pulse modification, mode-locking.

Practical lasers. Solid-state lasers, gas lasers, chemical and excimer lasers. Examples.

Applications of lasers in chemistry: Femtochemistry. The pump-probe technique. Time-resolved spectroscopy. Photodissociation of ICN. Formation and dissociation of CO-hemoglobin complex. Conversion of ethylene to cyclobutane. Bond selectivity in chemical reactions – the reaction between hydrogen atoms and vibrationally excited HDO molecules.

Lasers and multiphoton spectroscopy – underlying principles. Two-photon spectra of diphenyloctatetraene. Lasers in fluorescence spectroscopy and Raman spectroscopy.

Books suggested:

1. Modern Spectroscopy, J. M. Hollas, John Wiley & Sons
2. Fundamentals of Molecular Spectroscopy, Banwell & McCash
3. Introduction to Molecular Spectroscopy, G. M. Barrow, McGraw Hill
4. Molecular Spectroscopy, J. D. Graybeal, McGraw Hill
5. Basic principles of Spectroscopy, R. Chang, McGraw Hill
6. Physical Methods for Chemistry, R. S. Drago, Affiliated East West Press
7. Vibrational Spectroscopy: Theory and Applications, D. N. Sathyanarayana, New Age International
8. Introduction to Raman Spectroscopy, J. R. Ferraro & K. Nakamoto, Academic Press
9. NMR Spectroscopy: Basic principles, concepts and applications in chemistry, H. Gunther, John Wiley-VCH publishers
10. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, R. V. Parish, Ellis Harwood
11. NMR basic principles - Atta-ur-Rahman, Springer.
12. Two dimensional NMR Spectroscopy-Applications for chemists and biochemists, edited by W. R. Croasmun & R. M. K. Carlson, Wiley-VCH
13. X-ray diffraction procedures for polycrystalline and amorphous materials, H. P. Klug & L. E. Alexander, John Wiley
14. Physical Chemistry, Ira N. Levine, McGraw Hill
15. Atkin's Physical Chemistry, P. Atkins & Julio de Paula, Oxford University Press
16. A Guide to Lasers in Chemistry, G. R. Van Hecke & K. K. Karukstis, Jones and Bartlett Publishers
17. Lasers in Chemical and Biological Sciences, S. Chopra & H. M. Chawla, Wiley Eastern Ltd.
18. Molecular structure and Spectroscopy, G. Aruldas, Eastern Economic Edn.

ELECTIVE 3A**PAPER III CH(PC) 303T(CB1) : APPLIED CHEMISTRY, MATERIAL SCIENCE AND RADIATION EFFECTS**

PC(CB1)-1 : Applied kinetics

PC(CB1)-2 : Applied Electrochemistry

PC(CB1)-3 : Types of materials, conducting organics and NLO materials

PC(CB1)-4 : Radiation effects

PC(CB1)-1:Applied kinetics

(15 hrs)

Kinetics and chemical reaction engineering. Reactor design: Basic objectives in design of a reactor. Parameters affecting the reactor performance. Balance equations for reactor design. Single ideal reactor models.

Batch reactors (BR): General features. Design equations for a BR. Material and energy balances. Isothermal operation, constant-density system.

Continuous stirred-tank reactors (CSTR): General features. Design equations for a CSTR. Material and energy balances. Constant-density system. Steady-state operation at specified temperature. Damkohler number – numerical problems.

Plug-flow reactors (PFR): General features. Design equations for a PFR. Material and energy balances. Constant-density system.

Comparisons of ideal reactors for a single reaction. Single-vessel comparisons. BR and CSTR. BR and PFR. Numerical examples.

PC(CB1)-2:Applied Electrochemistry

(15 hrs)

Batteries: Battery parameters. Energy density power density and Ragone plot. Measures of battery performance. Primary and secondary batteries. Zn/MnO₂, lead-acid and Ni-Cd batteries and Lithium cells; Lithium-thionylchloride cell and lithium-ion battery.

Fuel cells: General Chemistry of Fuel cells. Types of fuel cells: H₂/O₂ and methanol/O₂ fuel cells. Use of porous electrodes in fuel cells. Advantages, limitations and efficiency of fuel cells.

Photovoltaic cells: Semiconductor based photoelectrochemical cells. Electrochemical energy from solar energy.

Anodic oxidation of metals. Characteristics of anodic oxide films. Industrial application of anodic oxide films.

Electroplating: Technical importance. Mechanism of electroplating. Alkaline and acid plating of copper, nickel.

Electro-organic synthesis: Reduction of carboxylic acids, the polymerization of acrylonitrile to adiponitriles in the synthesis of nylon. Reduction of nitro compounds.

PC(CB1)-3: Types of materials, Conducting Organics and NLO materials (15 hrs)

Classification of materials – metals, ceramics, polymers, composites, semiconductors and biomaterials.

Glassy state – glass formers and glass modifiers, applications

Ceramics – criteria for determining the crystal structure of ceramic materials – examples.

Composites – particle reinforced and fibre reinforced composites.

Preparative methods of solid materials - Ceramic method (Solid State method), co-precipitation as a precursor to solid state reaction, solutions and gels (Zeolite synthesis), crystallization from melts: Czochralski method, Kyropolous method; vapour phase transport method, modification of existing structure by ion-exchange and interaction reactions.

Techniques of single crystal growth – growth from solutions – growth from melts – growth from vapour. Non-linear optical (NLO) behavior– basic concepts, second and third harmonic generation, examples of organic, inorganic and polymer NLO materials.

Conducting organics – Fullerenes, alkali metal doped fullerides, fullerenes as superconductors

PC(CB1)-4: Radiation effects

15hrs

Radiation hazards and safety: Radiation effects. High-energy radiation and high-energy particles – types and sources. Radiation protecting materials.

Radiation chemistry of liquid water. Chemical yields. Dosimetry. Fricke dosimeter and thiocyanate dosimeter. Effect of radiation on DNA. Direct and indirect effects. Reaction of OH radicals with DNA constituents. General mechanism of strand break formation in DNA by OH radicals.

Radioactive wastemanagement: Introduction, Classification of radioactive waste, Treatment of Radioactive waste: Radioactive waste disposal.

Applications of radioisotopes in nuclear medicine and pharmaceuticals: general applications of radiopharmaceuticals, use of nuclear properties of indicator nuclides. In vivo diagnostic procedures, in vitro diagnostic testing therapeutic use of radiations, Use of radiation for food preservation and sterilization.

Books suggested:

1. Introduction to Chemical reaction Engineering and Kinetics, R. W. Missen, C. A. Mims & B. A. Saville, John Wiley
2. Chemical Reaction Engineering, O. Levenspiel, John Wiley
3. Chemical Engineering Kinetics, J. M. Smith, McGraw Hill
4. Elements of Chemical Reaction Engineering, H. Scott Fogler, Prentice Hall (page-114)
5. Modern Electrochemistry 2B, Bockris & Reddy, Plenum
6. Industrial Electrochemistry, D. Pletcher, Chapman & Hall
7. Introduction to Electrochemistry, S. Glasstone, EAST-WEST Press Pvt. Ltd, New Delhi
8. Electrochemistry – B K Sharma
9. Fundamental principles of Modern Electroplating, Lowenheim, John Wiley
10. The physics and chemistry of solids. Stephen Elliot, John Wiley & Sons
11. Solid state chemistry and applications. A.R. West, John Wiley & Sons

12. New directions in solid state chemistry. CNR Rao and Gopalakrishnan, Cambridge University Press
13. Principles of the Solid State, H. V. Keer, New Age International
14. Material Science and Engineering – An Introduction, William D. Callister, Jr., Wiley & Sons
15. Materials Science & Engineering – A First Course, V. Raghavan, Prentice Hall
16. Radiation Chemistry: Principles and Applications, Farhataziz and M. A. J. Rodgers (Eds.), VCH Publishers, New York (1987).
17. Radiation Chemistry: Present Status and Future Trends, C. D. Jonah and B. S. M. Rao (Eds.) Elsevier, Amsterdam (2001).
18. Essentials of Nuclear Chemistry: H. J. Arnikar. New Age Publication Ltd. (1995).
19. Radiation chemistry and Nuclear Methods of Analysis W. D. Ehmann, D. E. Vance. John Wiley (1991).
20. Nuclear and Radiochemistry G. Friedelarder, J. W. Kennedy, E. S. Macias, J. M. Miller John Wiley (1981).
21. Source Book of Atomic Energy, S. Glasstone, D. Van Nostrand (1967)
22. Nuclear analytical chemistry- J. Tolgyessy and S. Verga Vol. 2 , University park press (1972)
23. Fundamental of Radiochemistry, D.D.Sood, A.V.R.Reddy, N.Ramamoorthy, IANCAs , Mumbai, 4th Edition

ELECTIVE –3B

Paper III CH(PC) 303T(CB2) : BIOPOLYMER CHEMISTRY

PC(CB2)-5: Bioenergetics & physical properties of biopolymers

PC(CB2)-6: Biological membranes & binding of ligands by biopolymers

PC(CB2)-7: DNA, genes and cloning

PC(CB2)-8: Bioinformatics

PC(CB2)-5: Bioenergetics and physical properties of biopolymers

(15 hrs)

Bioenergetics: The standard state in biological processes. ATP – the currency of energy. Gibbs energy change in ATP hydrolysis, comparison with other phosphates. Principles of coupled reactions. Glycolysis and coupled reactions involving ATP. Biological oxidation-reduction reactions – transfer of H⁺ ions and electrons. Synthesis of ATP in the mitochondria. The chemiosmotic theory. Gibbs energy change accompanying the proton movement.

Viscometry: Molecular weights. Use of viscometry in the study of ligand binding to DNA. Separation/molecular weight studies of biopolymers. Light scattering method.

Sedimentation: Sedimentation velocity. Sedimentation coefficient. The Sverberg equation. Sedimentation equilibrium analysis. Ultra centrifugation Molecular weights. Light scattering method.

Electrophoresis : principle involved. Gel electrophoresis. Electrophoretic mobility. Applications.

PC(CB2)-6: Biological membranes and binding of ligands by biopolymers

(15 hrs)

Structure and function of cell membrane. Membrane equilibria and thermodynamics of membrane equilibria. Dialysis equilibrium. Osmotic pressure. Membrane potentials. Transport across membranes. Passive transport, facilitated transport and active transport.

Sodium-potassium pump. Selective ion transport and membrane potential. The Goldman equation (derivation not required). Nerve cells. The transfer of information in the body. The action potential and the mechanism of action potential propagation. Signal transducing mechanism involving gated ion channels in the plasma membrane.

Binding of ligands and metal ions to macromolecules – one and n-equivalent binding sites per molecule. Allosteric interactions – Oxygen binding to myoglobin and hemoglobin – Cooperative and non-cooperative binding. Hill equation and Hill plots. Transport of H^+ and CO_2 . Bohr effect.

PC(CB2)-7: DNA, genes and cloning

(15)hrs

Watson –Crick model of DNA. Types of DNA chains – linear, circular and supercoiled DNA. Types of RNA. Secondary structure of t-RNA

Genes and genome. Gene expression. Transcription and translation (general principles only). Codons and the genetic code. Sequence analysis of DNA by the Sanger chain-termination method.

Introduction to biotechnology and recombinant DNA technology. Molecular cloning. Restriction endonucleases and cloning vectors. Steps involved in the construction of recombinant DNA. DNA hybridization and hybridization probes.

Satellite DNAs – micro and mini satellites. Sequence polymorphisms – RFLPs. Principles of DNA finger printing technology.

PC(CB2)-8: Bioinformatics

(15 hrs)

Introduction: Use of informatics and computers in biology. Homology as descendants of common ancestors, statistical analysis of sequence alignment.

General purpose Databases for Comparative Genomics: COGs, KEGG, MDGB - Organism Specific Databases examples - E. Coli, Yeast, Oryza.

Introduction to Proteins - primary, secondary, tertiary and quaternary structures.

Structure databases – PDB, MMDB, CSD. Homology modeling – Flow chart, structure refinement - Ramachandra Plot.

Books suggested:

1. Biophysical Chemistry, Cantor & Schimmel, W. H. Freeman and Company
2. Principles of Physical Biochemistry, Kensal E van Holde, W. Curtis Johnson & P. Shing Ho, Prentice Hall
3. Physical Biochemistry : Principles and Applications, David Sheehan, John Wiley
4. Physical Chemistry for the Chemical and Biological Sciences, Raymond Chang, University Science Books
5. Lehninger Principles of Biochemistry, D. L. Nelson & M. M. Cox, MacMillan
6. Biochemistry, L. Stryer, W. H. Freeman and Company
7. Concepts in Biochemistry, Rodney Boyer, Books/Cole Publishing Company
8. Modern Electrochemistry 2B, Bockris & Reddy, Kluwer Academic/ Plenum
9. Introduction to Bioinformatics by Arthur Lesk, Oxford University Press, Inc, New York
10. Bioinformatics, A practical guide to the Genes and Proteins. Edited by Andreas. D. Baxeavanis and B. F. Francis Wiley Publishers

ELECTIVE 4A**Paper IV CH(PC) 304T(CB3) :POLYMER CHEMISTRY**

PC(CB3)-9: Polymerization and Kinetics of polymerization

PC(CB3)-10: Structure and properties of polymers

PC(CB3)-11: Processing of Polymers

PC(CB3)-12: Functional polymers

PC(CB3)-9: Polymerization and Kinetics of polymerization

(15 hrs)

Classification of polymers. Types of polymerization.

Kinetics and mechanism of free radical polymerization. Degree of polymerization, kinetic chain length and chain transfer coefficient – Trommsdorff effect. Effect of pressure and temperature on chain polymerization.

Kinetics and mechanism of cationic, anionic polymerization, coordination polymerization, linear stepwise polymerization.

copolymerization reactions and copolymer composition. Reactivity ratios and their determination. Alfrey and Price Q-e scheme for monomer and radical reactivity. Block and graft copolymers.

Polymerization in homogeneous and heterogeneous systems. Techniques of polymerization-Bulk, solution, suspension and emulsion polymerizations.

PC(CB3)-10: Structure and properties of polymers

(15 hrs)

Polymer solutions:

The process of polymer dissolution. Thermodynamics of polymer dissolution. Entropy, heat and free energy of mixing of polymer solutions. Conformations of dissolved polymer chains. The freely jointed chain. Short-range and long-range interactions. The Flory-Huggins theory of polymer solutions. Dilute polymer solutions. Flory-Krigbaum theory.

Mechanical properties of polymers:

The elastic state. Rubber-like elasticity and viscoelasticity. Newtonian and non-Newtonian behaviour. Maxwell and Voigt-Kelvin models of viscoelastic behaviour.

The crystal structure of polymers. Morphology of crystalline polymers. Crystallization and melting. Determination of T_m . Thermodynamics of crystalline melting. Heats and entropies of fusion. Degree of crystallinity. Factors affecting the crystallization.

The glassy state – glass transition temperature T_g of polymers. Factors influencing T_g . Glass transition temperature and melting point.

Molecular weight distribution – measurement of molecular weights by end group analysis, osmometry and GPC.

PC(CB3)-11: Processing of Polymers

(15hrs)

General applications of Polymers. Polymer Additives - Fillers, plasticizers, lubricants, catalysts, stabilizers, colorants, antioxidants, flame retardents.

Processing techniques of polymers - (one dimensional coating -Adhesives, Lamination; extrusion- calendering and thermoforming ; Molding of Polymers- Process.) (advantages and limitations of Compression molding, Injection Molding, Extrusion Molding, Blow Molding)

Casting -(Types, Vacuum Casting, Potting, Encapsulation, Film Casting).

Fibre Reinforced Plastics- preparation and properties. Synthetic Fibres- Rayons, (Nitro cellular, Cupammonium, Diacetate, Viscose), Nylons, Dacron.

Processing of fiber reinforced Composites- Pultrusion technique, prepreg production processes, filament winding.

PC(CB3)-12: Functional polymers

(15hrs)

Smart materials – Their uses in sensing devices and in communication networks.

Electrically conducting polymers- Introduction, basic principles and their applications. Brief description of polyanilines, polypyrrole, polyacetylene and polythiophene.

Photoconductive polymers, Liquid crystal polymers – smectic, nematic and cholesteric structures, Ionic exchange polymers- Cationic and anionic exchange polymers and their uses.

Biodegradable polymers- Definition, classification, applications. Brief description of polyhydroxyalkanoates, polycaprolactone, polyacetic acid and polyvinylalcohol.

Polymers in Membrane separation. Filtration – micro, ultra and nanofiltration. Separation of gases – permeselectivity and gas permeability of representative polymers. Liquid separation – dialysis, electro osmosis and reverse osmosis.

Fire retarding polymers, photonic polymers.

Polymers in biomedical applications – artificial organs and controlled drug delivery.

Books suggested:

1. Textbook of Polymer Science, F. W. Billmeyer Jr, John Wiley & sons
2. Polymer Science, V. R. Gowarikar, N. V. Viswanathan & J. Sreedhar, Wiley Eastern
3. Contemporary Polymer Chemistry, H. R. Alcock & F. W. Lambe, Prentice Hall
4. Physics and Chemistry of Polymers, J. M. G. Cowie, Blackie
Academic and professional
5. Materials science and engineering an introduction by William D Callister, Jr. Wiley Publishers
6. Polymer Chemistry, B. Vollmert, Springer publishers
7. Physical Chemistry of Polymers, A. Tagers, Mir Publishers
8. A text book of polymers, Vol. I,II,III, M.S. Bhatnagar, S. Chand publishers

ELECTIVE 4B**Paper IV CH(PC) 304T(CB4) : ENVIRONMENTAL CHEMISTRY**

PC(CB4)-13: Pollution in Atmosphere

PC(CB4)-14: Pollution in Hydrosphere

PC(CB4)-15: Heavy Metal and Radiochemical Pollution.

PC(CB4)-16: Analysis of Air, Water and Metal Pollutants

PC(CB4)-13: Pollution in Atmosphere

Typical Composition of Unpolluted Dry Air - Major Air Pollutants: Carbon Monoxide, Nitrogen Oxides, Sulphur Oxides, Particulate Matter, Hydrocarbons, Chlorofluorocarbons.

Carbon Monoxide: Sources and Sinks, Concentration Profile, Effects on Human Health, Control of CO Emissions.

Nitrogen Oxides (NO_x): Reactions Leading to Formation of NO_x, Sources and Sinks, Concentration Profile, Harmful Effects of NO_x on Human Beings, Plants, Materials and Control of NO_x Emissions.

Sulphur Oxides (SO_x): Reactions Leading to Formation of SO_x, Sources of SO_x. Harmful Effects on Human Beings, Plants and Materials - Control of SO_x Emissions - Acid Rain: Formation and Toxic Environmental Effects.

Particulate Matter: Sources, Inorganic and Organic Particulate Matter - Effects on Human Beings, Materials and Climate - Control of Particulate Emissions.

Hydrocarbons: Sources - Types of Polluting Hydrocarbons - Hydrocarbons and Photochemical Smog Formation - Harmful Effects of Photochemical Smog - Control of Hydrocarbon Emissions .

Green House Effect: Causes, Consequences and Abatement of Green House Effect - Ozone Depletion - Mechanism, Causes, Consequences and Abatement of Ozone Depletion - Bhopal Gas Tragedy and Sevozo Disaster.

PC(CB4)-14: Pollution in Hydrosphere

Types of Water Pollutants and their Effects - Sources of Water Pollution: Domestic, Industrial, Agricultural, Soil, Thermal and Radioactive Wastes - Types of Persistent Pollutants - Biomagnification of Persistent Pollutants, Effects of Biomagnified Pollutants on Human Beings (DDT) – Triphosphates: Their Role in Eutrophication of Water Bodies - Ecological Consequences of Eutrophication, Bacteriological Contamination of Water - Dissolved Oxygen in Natural Waters - Depletion of Dissolved Oxygen - Biological Oxygen Demand and Chemical Oxygen Demand as Indicators of Extent of Water Pollution - Nitrates, Nitrites, Nitrosoamines in Water: Their Toxic Effects On Human Beings - Treatment of Drinking Water Supplies.

PC(CB4)-15: Heavy Metal and Radiochemical Pollution.

Essential and Toxic Elements in Nature - Mechanism of Metal Ion Toxicity - Effects on Non-Metalloenzymes, Metalloenzymes, Cell Membranes, Nucleic Acids - Concepts of Speciation, Biomethylation and Biomagnification.

Mercury: Sources of Pollution. Speciation and Environmental Forms of Mercury - Biochemical Effects of Different Species of Mercury - Minamata Bay Episode as a Case Study of Mercury Poisoning.

Arsenic: Sources of Pollution - Speciation and Environmental Chemistry of Arsenic - Biochemical Effects of Different Species of Arsenic.

Lead: Sources of Lead Pollution - Speciation and Pathways of Lead in Environment - Biochemical Effects of Lead.

Cadmium: Sources of Pollution – Speciation - Biochemical Effects of Cadmium Poisoning.
Radiochemical Pollution: Sources, Chemical Changes due to Radiation on Water.

Organic Compounds - Harmful Effects of Radioactive Pollutants on Living Organisms - Permissible Limits of Radiation - Control and Disposal of Radioactive Wastes - Chernobyl Disaster.

PC(CB4)-16: Analysis of Air, Water and Metal Pollutants

Air Quality Standards - Sampling (Particulates and Gaseous Pollutants) - Analysis of Pollutants: SO₂ (Modified West-Gaeke Spectrophotometric Method, Pulsed Fluorescence Spectrometry), H₂S (Spectrophotometry – Ethylene Blue Method), NO-NO_x (Chemiluminescence Technique, Colorimetric Technique- Saltzman Method) – CO (NDIR Spectrometry, GC), Hydrocarbons (Ionization Analysis), Aromatic Hydrocarbons in Automobile Exhausts, Petrol, Air, O₃ (Chemiluminescence and Spectrophotometry) - Particulate Matter Analysis (High Volume Method).

Water Sampling, Preservation and Preconcentration Methods and Physical Analysis - Colour, Odour, Temperature, pH, EC, Redox Potential and Total Dissolved Solids (Turbidimetry). Chemical Analysis of Anions: CN⁻, Cl⁻, F⁻ (Spectrophotometry, Ion Selective Potentiometry and Titrimetry), NO₂⁻ and NO₃⁻ (Spectrophotometry), SO₄²⁻, PO₄³⁻, HCO₃⁻, CO₃²⁻, Hardness of Water (Titrimetry), Ammonical Nitrogen (Spectrophotometry) - Determination of DO, BOD, COD, TOC in Water.

Books Suggested:

1. Environmental Chemistry, John. W. Moore and Elizabeth Moore Academic press New York
2. Principles of Environmental Chemistry, Stanley E. Manahan 2nd Ed.
3. Environmental Chemistry, 4th ed. A.K. De. New Age International Publishers, 2000
4. Environmental Pollution Analysis, S.M. Khopkar Wiley Eastern Ltd. 1995
5. Environmental Chemistry, Colin Baird W.H. Freeman and Company New York 1995.
6. Text Book of Environmental Chemistry, Ayodhya Singh, Campus Books International publishers
7. Chemistry of the Environment, II Edn Thomas G.Spiro William M.Stigliani
8. Fundamental Concepts of Environmental Chemistry, G.S.Sodhi Narosa Publishing House.
9. Environmental Analytical Chemistry, F.W.Fifield,P.J.Haines,Blackie Academic & Professional

III SEMESTER PRACTICALS

CH (PC) 351 P: Paper-V (Chemical Kinetics)

9 hrs/week

Note: The data obtained in all the experiments are to be analyzed by the students both *by the usual graphical methods and by regression (linear/nonlinear) techniques using a PC.*

- ◆ Study of peroxydisulphate – iodide reaction:
 1. Individual orders of the reactants by initial rate and isolation methods
 2. Effect of temperature on reaction rate
 3. Effect of ionic strength on reaction rate
- ◆ Study of peroxydisulphate – iodide clock reaction:
 1. Individual orders of the reactants ,
 2. effect of ionic strength on uncatalyzed and Cu(II)-catalyzed reactions
- ◆ Study of acetone – iodine reaction by titrimetry
 1. Order w.r.t.[iodine]
 2. Order w.r.t. [acetone]
 3. Order w.r.t. [H⁺]

CH (PC) 352 : Paper-VI (Instrumentation)

9 hrs/ week

Conductometry:

- ◆ Conductometric titrations:
 1. Mixture of strong and weak bases vs strong acid
 2. Mixture of strong and weak acids vs weak base
 3. Mixture of strong acid, weak acid and CuSO₄ vs strong base
 4. Mixture of halides (chloride + iodide) vs AgNO₃
 5. Formic acid, acetic acid, chloroacetic acid, dichloroacetic acid and Trichloroacetic acid
 6. and their mixtures vs strong base
 7. Precipitation titration: K₂SO₄ vs BaCl₂
- ◆ Dissociation constants of weak acids
- ◆ Effect of solvent on dissociation constant of a weak acid
- ◆ Verification of Onsager equation
- ◆ Composition of Cu(II) – tartaric acid complex by Job's method

pH metry:

- ◆ pH – metric titrations:
 1. Monobasic acids vs strong base
 2. Dibasic acid vs strong base
 3. Tribasic acid vs strong base
 4. Mixture of strong and weak acids vs strong base
- ◆ Determination of dissociation constants of monobasic/dibasic acids by Albert- Serjeant method
- ◆ Determination of dissociation constant of acetic acid in DMSO, acetone and dioxane
- ◆ Determination of pK_a and pK_b of glycine (calculation using a computer program)
- ◆ Determination of stability constant of a metal complex

Suggested books:

1. A textbook of practical organic chemistry by A I Vogel, Vol 1&2.
2. Senior practical physical chemistry. B. D. Khosla, V.C. Garg, Adarsh Gulati
3. Experimental Physical Chemistry: V. Athawale and P. Mathur.
4. Practical Physical Chemistry: B. Vishwanathan and P.S. Raghavan.
5. Practical in Physical Chemistry: P.S. Sindhu
6. Advanced Practical Physical chemistry: J.B. Yadav

M.Sc. SEMESTER - IV
PHYSICAL CHEMISTRY SPECIALIZATION
(For the batches admitted in academic year 2016 and later under CBCS pattern)

PAPER I CH(PC)401: Thermodynamics, Chemical kinetics and Electrochemistry

PC-17 : Statistical Thermodynamics
 PC-18 : Non-equilibrium Thermodynamics
 PC-19 : Chemical Kinetics-II
 PC-20 : Electrochemistry -II

PC -17: Statistical Thermodynamics (15 hrs)

Concepts of distribution and probability. Estimation of probability and the most probable distribution. Systems composed of noninteracting particles. Derivation of Boltzmann distribution law. The molecular partition function. Systems composed of interacting particles.

The concept of ensemble and canonical ensemble. Canonical partition function and its relation to molecular partition function. The factorization of molecular partition function – translational, rotational, vibrational and electronic partition functions. Derivation of expressions for translational, rotational (diatomic) and vibrational partition functions. Relationship between partition functions and thermodynamic functions. The relationship between partition functions and thermodynamic functions. Law of equipartition energy.

Specific heats of solids – Einstein equation of heat capacity of solids – derivation. Explanation of heat capacity at very low and very high temperatures – Dulong and Petits Law. Debye theory. The entropy of a monoatomic ideal gas. The Sackur-Tetrode equation- derivation. Mean translational and vibrational energies.

The relation between equilibrium constant and partition function- derivation.

Basic ideas of Bose-Einstein statistics and Fermi-Dirac statistics and comparison of these with Maxwell-Boltzmann statistics.

PC-18: Non-equilibrium Thermodynamics (15hrs)

Thermodynamic criteria for non-equilibrium states. Entropy production in irreversible processes. Entropy production in heat flow and entropy production in material flow.

Fluxes and forces. Linear flux-force relations. Phenomenological equations and coefficients. Microscopic reversibility. Onsager reciprocal relations.

Application of Onsager relations to electrokinetic phenomena – electroosmotic pressure and streaming current. The Onsager relations and the principle of detailed balance. Liquid junction potentials – derivation of equation for liquid junction potential in terms of transport numbers using Onsager relations. Steady states. Principle of minimum entropy production.

Irreversible thermodynamics as applied to biological systems - examples.

Application to thermoelectric circuits. Seebeck and Peltier effect.

PC-19: Chemical kinetics – II:

(15hrs)

Reactions in solution: Factors affecting reaction rates in solution. Effect of pressure on rate of reaction. Diffusion controlled reactions. Influence of dielectric constant and ionic strength on ion-ion, ion-dipole and dipole-dipole reactions. Primary and secondary salt effects. Kinetic isotope effects: Primary and secondary isotope effects. Solvent isotope effects.

Fast reactions: Flow methods and the stopped-flow technique. The fluorescence technique. Shock tube method. Relaxation methods (T-jump and P-jump). Kinetic equations for chemical relaxation.

Enzyme kinetics: Michaelis - Menten mechanisms of enzyme catalyzed reactions involving one and two intermediates. Steady-state approximation. Derivation of kinetic equations. Evaluation of kinetic parameters. Enzyme- substrate complex: Fischer's lock and key and Koshland's induced fit hypotheses. Specificity of enzyme-catalyzed reactions. Discussion of the various types of forces involved in the formation of E-S complex. pH dependence of enzyme-catalyzed reactions – the kinetics and the equations involved.

PC –20 : Electrochemistry – II

(15 hrs)

The electrode-electrolyte interface: The electrical double layer. The Helmholtz-Perrin parallel-plate model, the Gouy-Chapman diffuse-charge model and the Stern model. Quantum aspects of charge transfer at the interfaces. Tunneling.

Electrodics: Charge transfer reactions at the electrode-electrolyte interface. Exchange current density and overpotential. Derivation of Butler-Volmer equation. High field approximation. Tafel equation - low field - equilibrium, Nernst equation. The symmetry factor and its significance.

Corrosion: Electrochemical corrosion. Short-circuited energy producing cell. The definition and final expression of corrosion current and corrosion potential. Homogeneous theory of corrosion. Evans diagrams. Potential-pH (Pourbaix) diagrams of iron. Methods of corrosion rate measurement. Mechanism of anodic dissolution of iron. Protection against corrosion. Corrosion inhibition by organic molecules.

Books suggested:

1. Elements of Statistical Thermodynamics, L. K. Nash, Addison – Wesley
2. Introduction to Statistical Thermodynamics, T. L. Hill, Addison Wiley
3. Statistical Thermodynamics, M. C. Gupta, New Age International
4. Atkin's Physical Chemistry, P. Atkins & Julio de Paula, Oxford University Press
5. Molecular Thermodynamics, D. A. McQuarrie & J. D. Simon, University Science Books
6. Text book of Biochemistry by Stryer, W.H. Freeman & Co Ltd
7. Advanced physical chemistry by Gurtu and Gurtu, Pragati Edition
8. Physical chemistry by Puri and Sharma, Vishal Publishing Co.
9. Chemical Kinetics, K. J. Laidler, McGraw Hill
10. Kinetics and Mechanism, A. A. Frost & R. G. Pearson, John Wiley & sons
11. Kinetics and Mechanism of Chemical Transformations, J. Rajaraman & J. Kuriacose, McMillan
12. Chemical Kinetics and Reaction Mechanisms, J. H. Espenson, McGraw Hill
13. Physical Organic Chemistry, N. S. Isaacs, ELBS

14. The Physical basis of Organic Chemistry, Howard Maskill, Oxford University Press
 15. Modern Electrochemistry, J. O. M. Bockris & A. K. N. Reddy, Plenum.
 16. Modern Electrochemistry 2B, Bockris & Reddy, Plenum.
 17. Introduction to Electrochemistry, S. Glasstone, EAST-WEST Press Pvt. Ltd, New Delhi

PAPER- CH(PC) 402T: SUPRAMOLECULAR CHEMISTRY, PHOTO CHEMISTRY AND COMPUTATIONAL CHEMISTRY

- PC-21 : Supramolecular Chemistry
 PC-22 : Photochemistry
 PC-23 : Computational Chemistry
 PC-24 : Theoretical treatment of bio polymers

PC-21: Supramolecular Chemistry

Concepts: Molecules, super molecules and supramolecules. Nature of Supramolecular interactions.

Molecular recognition – factors involved. Ionophores. Molecular receptors – design principles.

Molecular receptors for alkali metal ions, ammonium ions, anions and neutral molecules. Crown ethers, cryptands, spherands, calixaranes, and cyclodextrins – their selectivity, macrocyclic, and template effects. Fullerenes as supramolecules.

Threading of a linear molecule through a cyclic molecule – creation of Rotaxanes and Catenanes.

Thermodynamics of host-guest complexation. Enthalpy and entropy contributions. Complexation free energies.

Supramolecular catalysis- Crownether supported alkaline earth metal ions as catalysts, cyclodextrins and calixaranes as catalysts in chemical reactions. Transport of ions across membranes by biological molecules.

Molecular electronic devices: Molecular wires, molecular switches and machines.

PC-22: (Photochemistry – I)

(Formation) of excimers and exciplexes – PE diagram and quantum yields. Energy transfer mechanism for bimolecular quenching. Long-range coulombic energy transfer – critical transfer distance. Short-range electron exchange energy transfer. Triplet-triplet energy transfer and sensitization.

P-type delayed fluorescence. The experimental study of photochemical reactions: Product analysis, chemical methods in the study of intermediates, spectroscopic methods, ESR and CIDNP, rate coefficients for photochemical processes and identification of excited states.

Electronic transitions in transition metal complexes. Ligand field (LF) and charge transfer (CT) electronic states. $\text{Ru}(\text{bpy})_3^{2+}$ as sensitizer for photoredox reactions, examples. Photochemical cleavage of water.

PC-23: Computational treatment of many electron systems

(15hrs)

Multi-electron atoms. The antisymmetry principle and the Slater determinant. The Hartree-Fock method. The Hartree-Fock equations.(no derivation). The Fock operator. Core hamiltonian. Coulomb operator and exchange operator. Slater-type orbitals (STOs) as basis functions. Orbital energies and total energy. Helium atom example. Koopman's theorem. Hund's rules and theoretical basis of the Aufbau principle. Electron correlation energy.

The Hartree-Fock method for molecules. Restricted and unrestricted HF calculations. The Roothan equations. The Fock matrix. The Roothan matrix elements. GTOs and different types of basis sets. Minimal basis set. Model HF calculations on H₂. Discussion of results of HF calculations on simple molecules – H₂O and NH₃. Introduction to configuration interaction.

Density functional theory (DFT). Hohenberg-Kohn theorem. Kohn-Sham (KS) formulation of DFT. KS equations and KS orbitals. Brief explanation of exchange-correlation energy and exchange- correlation potential.

PC-24: Theoretical treatment of biopolymers

(15 hrs)

Types of biopolymers. Methods of determining Size and shape of biopolymers - mean molecular masses, colligative properties, sedimentation, viscosity, light scattering methods.

Chain conformation and configuration of poly peptides. Random coils and measures of size – contour length, rms separation, radius of gyration, constrained chains.

Secondary structures of proteins- helices and sheets: The Corey-Pauling rules. Conformational energy of a polypeptide- bonding, nonbonding potentials, electrostatic interactions, dipole-dipole interactions and van der Waals interactions. Hydrogen bonds. Principles of molecular mechanics to calculate potential energy of a polypeptide. Ramachandran plots of α -helix and β -sheet.

Conformational entropy. Introductory treatment of the protein folding problem.

Books suggested:

- 1) J.W Steed and J.L Atwood, Supramolecular chemistry, John Wiley & Sons, Ltd. New York.
- 2) Piet W. N. M. van Leeuwen, Supramolecular Catalysis, Wiley-VCH Verlag GmbH & Co.
- 3) Principles and methods in supramolecular chemistry, Hans-Jorg Schneider and A.Yatsimirsky, John Wiley and Sons.
- 4) Analytical Chemistry of Macrocyclic and Supramolecular Compounds, S.M.Khopkar, Narosa Publishing House
- 5) Essentials of Molecular Photochemistry, A. Gilbert & J. Baggott, Blackwell Science
- 6) Quantum Chemistry, I. N. Levine, Prentice Hall
- 7) Molecular Quantum Mechanics, P. W. Atkins and R. S. Friedman, Oxford University Press
- 8) Introduction to Computational Chemistry, F. Jensen, John Wiley & Sons
- 9) Elementary Quantum Chemistry, F. L. Pilar, McGraw Hill
- 10) Modern Quantum Chemistry, A. Szabo and N. S. Ostlund, Dover publishers
- 11) Computational Chemistry: Introduction to the theory and Applications of Molecular and Quantum Mechanics, Errol Lewars, Springer Publications
- 12) Physical Chemistry, D. A. McQuarrie and J. D. Simon, Viva Books Ltd.
- 13) Physical Chemistry, P. W. Atkins, Oxford Unibersity Press.

- 14) Approximate Molecular Orbital Theory, J. A. Pople and D. L. Beveridge, McGraw Hill
 15) Biophysical Chemistry, Cantor & Schimmel, W. H. Freeman and Company
 16) Principles of Physical Biochemistry, Kensal E van Holde, W. Curtis Johnson & P. Shing Ho, Prentice Hall
 17) Physical Biochemistry : Principles and Applications, David Sheehan, John Wiley
 18) Physical Chemistry for the Chemical and Biological Sciences, Raymond Chang, University Science Books

ELECTIVE –3A:

PAPER III CH(PC)- 403T(CB1): CATALYSIS

- PC(CB1)-17: Homogeneous catalysis
 PC(CB1)-18: Surface Chemistry & Micellar catalysis
 PC(CB1)-19: Heterogeneous catalysis
 PC(CB1)-20: Phase transfer , Anchored & Photo catalysis

PC(CB1)-17: Homogeneous catalysis

(15 hrs)

Introduction to catalysis. Types of catalysis, characteristics of catalyst, catalyst supports, promoters, general mechanism of catalysis, equilibrium treatment and steady state treatment. Activation energies of catalyzed reactions.

Acid-base catalysis, specific acid-base catalysis, general acid base catalysis, mechanism of acid – base catalysis, catalytic activity and acid-base strength- Bronsted relationships.

Acidity functions: Types of acidity functions. Hammett acidity function. Measurement of Hammett acidity function(H_0), usefulness of Hammett acidity function in understanding the mechanism of an acid catalyzed reactions. Zucker-Hammett hypothesis and its applications. Bunnett – Olson’s criteria of acid-base catalyzed reactions with examples.

Catalysis by transition metal ions and their complexes. Use of Ziegler –Natta and metallocene catalysts as homogeneous catalysts for polymerization of olefins. Application of metal ion catalysis to the hydrogenation of alkenes, hydroformylation, oxidation and isomerization reactions. Asymmetric Catalysis–Introduction, Catalysts, Commercial Applications, Asymmetric Hydrogenation, Enantioselective Isomerization: L-Menthol, Asymmetric Epoxidation.

PC(CB1)-18: Surface Chemistry and Micellar catalysis

(15hrs)

Surface tension. Curved interfaces. The Laplace equation. Capillary action. Thermodynamics of surface layers – Gibbs isotherm.

Adsorption. Types of adsorption, factors effecting adsorption, Chemistry and thermodynamics of adsorption. Determination of heats and entropies of adsorption.

Surface versus bulk structures. Adsorbate -induced restructuring of surfaces. Thermal activation of bond breaking on a surface. Co-adsorption. Chemisorption isotherms. Kinetics of chemisorption.

Surface films. Monometallic surfaces and bimetallic surfaces. Experimental techniques for the study of monolayer films. States and reaction in monomolecular films. Reaction between $H_2(g)$ and $N_2(g)$ catalyzed by surfaces to give $NH_3(g)$.

Micelles: Classification of surface active agents. Micellization and micellar interactions. Structure of micelles – spherical and lamellar. Critical micellar concentration (CMC). Factors affecting the CMC of surfactants.

Counter ion binding to micelles. Thermodynamics of micellization. Phase separation and mass action models, solubilization, micro emulsion, reverse micelles. Reactions assisted by micelle formation. Examples of micelle-catalyzed reactions and their mechanisms.

PC(CB1)-19: Heterogeneous catalysis

(15 hrs)

Heterogeneous catalysis. Broad categories of catalysts – metals, bimetals, semiconductors, insulators, zeolites, oxides, nano materials.

Preparation of metal catalysts, supported metal catalysts and non-metallic catalysts. Coprecipitation, Impregnation, sol-gel method, deposition-precipitation, hydrothermal synthesis, pulsed laser methods, plasma chemical methods, chemical vapor deposition methods

Steps in heterogeneous catalyzed reactions. Diffusion and adsorption. Mechanism of surface-catalyzed reactions. Adsorption isotherms - Langmuir Hinshelwood model, Rideal - Eley mechanism, Kinetics and thermodynamics of catalysed reactions. Catalytic activity – the determining factors. Structure sensitive and structure insensitive catalysts.

Characterization of catalysts: Surface area by BET method. Determination of pore volume and pore size distribution by BJH method. Pore size and specificity of catalysts. Surface acidity of catalysts- Determination of surface acidity by indicator method, IR spectroscopic method and TPD methods. Surface characterization by XRD, LEED, TEM & AFM, XPS, AES, techniques.

Auto exhaust emissions- catalytic converters. Catalytic hydrogenation and oxidation reactions.

Cracking and reforming. Fischer-Tropsch synthesis of methanol.

PC(CB1)-20: Phase transfer, Anchored and Photo catalysis

(15 hrs)

Phase-transfer catalysis (PTC): Principles of phase-transfer catalysis. PTC classification.

Role of water in phase-transfer catalyzed reactions. Factors influencing the rate of PTC reactions.

Inverse phase transfer catalysis. Mechanism of nucleophilic displacement reactions.

Crown ethers: Crown ethers as phase transfer catalysts(PTC) in the reaction of alkyl halides with super oxide. Permanganate oxidation of alkenes and phenols in presence of PTC's viz., quaternary ammonium salts and crown ethers.

Anchored catalysis: Definition and examples of anchored catalysis- organic polymers, inorganic oxides and clays as supports. Structure of montmorillonite anchored catalysts- HEW structure and EF structure. Montmorillonite anchored catalysts- application of intercalated clay catalysts in hydrogenation reactions.

Photo catalysis: Photocatalytic effect, metal semiconductor systems as photo catalysts, nature of the metal loaded, extent of metal loading, nature of semiconductor, doped semiconductors, coupled Semiconductors. Application of photocatalysis for splitting of water by semiconductor particles, removal of organic and inorganic pollutants, for oxidation and reduction of organic compounds.

Books suggested:

1. Principles of Heterogeneous Catalysis in practice, G. C. Bond, Oxford Publishing
2. Heterogeneous Catalysis, C. Satterfield, McGraw Hill
3. Catalysis, Principles and applications, edited by B. Vishwanathan, S. Sivasanker & A. V. Rama Swamy, Narosa Publishing House
4. Catalysis, J. C. Kuriacose, Macmillan
5. Colloidal and surface chemistry, M. Satake, Y. Hayashi, Y. Mido, S.A. Iqbal and M.S. Sethi
6. "Physical Organic Chemistry" by L.P. Hammett, chapter 9, McGraw Hill.
7. Chemical Review, **57**, 1935(1957), M.A. Paul and F.A. Long
8. Phase Transfer Catalysis, Fundamentals, Applications and Industrial perspective, C. M. Stark, C. Liotta & M. Halpern, Academic Press
9. Phase Transfer Catalysis, E. V. Dehmlow & S. S. Dehmlow, Verlag Chemie, Weinheim
10. Phase Transfer Catalysis in Organic synthesis, W. P. Weber & G. W. Gokel, Springer
11. Hand book of phase transfer catalysis Edited by Y. Sasson and R. Neumann
12. Catalysis in Micellar and Macromolecular systems, J. H. Feudler & E. J. Feudler, Acad. Press
13. Reaction Kinetics in Micelles, E. H. Codes (ed), Plenum
14. Micelles – Theoretical and Applied aspects, V. Moroi, plenum
15. Physical Chemistry of surfaces, A.W. Adamson and A.P. Gast, Wiley
16. Polymer supported Catalysts, C. U. Pittman Jr, vol 8, Comprehensive Organometallic Chemistry
17. Principles and Practice of Heterogeneous Catalysis, J. M. Thomas and W.J. Thomas, VCH 1997.
18. Spectroscopy in catalysis – An introduction by J. W. Niemantsverdriet.
19. Modern methods of Organic Synthesis: Ahluwalia.

ELECTIVE-3B**PAPER IV CH(PC) 403 T(CB2) : Dynamics of Chemical Reactions And Sensors**

PC-(CB2)-21: MO and VB theory of reactivity

PC-(CB2)-22: Kinetic, isotopic, structural, solvent, steric and conformational effects

PC-(CB2)-23: Nucleophilic, electrophilic and free radical reactivity

PC-(CB2)-24: Sensors

PC-(CB2)-21: Molecular Orbital (MO) and Valence Bond (VB) theory of reactivity 15 Hrs

Introduction to Huckel molecular orbital (MO) method as a means to explain modern theoretical methods. Advanced techniques in PMO and FMO theory. Molecular mechanics, semiempirical methods and ab initio and density functional methods. Scope and limitations of several computational programmes. Quantitative MO theory-Huckel molecular orbital (HMO) method as applied to ethane energy levels. Orbital symmetry, orbital interaction diagrams. MO of simple organic systems such as ethane, allyl, butadiene, methane and methyl group. Conjugation and hyperconjugation. Aromaticity. Valence bond (VB) configuration mixing diagrams. Relationship between VB configuration mixing and resonance theory. Reaction profiles. Potential energy diagrams. Curve crossing model nature of activation barrier in chemical reactions. Principle of reactivity Mechanistic significance of entropy, enthalpy and Gibbs free energy. Arrhenius equation, transition state theory. Uses of activation parameters.

PC-(CB2)-22: Kinetic, isotopic, structural, solvent, steric and conformational effects 15 Hrs

Theory of isotope effects, Primary and secondary kinetic isotope effects. Heavy isotope effects. Tunneling effect Solvent effects. Structural effects on reactivity: Linear free energy relationship (LFER.). The Hammett equation, substituent constants, theories of substituent effects. interpretation of σ -values. Reaction constant ρ . Deviations from Hammett equation. Dual—parameter correlations, inductive substituent constant The Taft model, σ_1 , σ_R scales. Solvation and solvent effects: Qualitative understanding of solvent- solute effects on reactivity Thermodynamic measure of solvation. Effects of solvation on reaction and equilibrium. Various empirical indexes of solvation based on physical properties, solvent- sensitive reaction rates, spectroscopic properties and scales for specific solvation. Use of solvation scales in mechanistic studies. Solvent effects from the curve-crossing model. Various type of steric strain and their influence on reactivity. Steric acceleration. Molecular measurements of steric effects upon rates. Steric LFER. Conformational barrier to bond rotation-spectroscopic detection of individual conformers. Acyclic and monocyclic systems. Rotation around partial double bonds. Winstein-Holness and Curtin-Hammet principle.

PC-(CB2)-23: NUCLEOPHILIC, ELECTROPHILIC AND FREE RADICAL REACTIVITY

15 Hrs

Bases, nucleophiles, Electrophiles and Catalysts. Acid-base dissociation. Electronic and structural effects, acidity and basicity. Acidity functions and their applications. Hard and soft acids and bases. Nucleophilicity scales, Nucleofugacity. The α -effect.- Ambivalent nucleophiles. Acid-base catalysis. Specific and general catalysis. Bronsted catalysis. nucleophilic and electrophilic catalysis. Catalysis by non-covalent binding micellar catalysts. Nucleophilic and electrophilic Reactivity:Structural and electronic effects on SN1 and SN2 reactivity. Solvent effects,kinetic isotope effects. Intramolecular assistance. Electron transfer nature of SN2 reaction. Nuclcophilicity and S2 reactivity based on curve-crossing model. Relationship between polar and electron transfer reactions. SRN1 mechanism. Electrophilic reactivity, general mechanism. Kinetics of SE2-Ar reaction, Structural effects on rates and selectivity. Curve crossing approach to electrophilic reactivity. ; Radical and pericyclic reactivity. (a)Radical stability, polar influences, solvent and steric effects. A curve crossing approach to radical addition, factors affecting barrier heights in additions, regioselectivity in radical reactions. Reactivity, specificity and periselectivity in pericyclic reactions.

PC-(CB2)-24: Chemical, Electrochemical and Bio Sensors

15hrs

Importance of Sensors, Biomolecular recognition elements, Artificial molecular-recognition materials, Molecular imprinted polymers, Electrode modification. Fluorescence, chemi and bioluminescence sensors, Fluorescent tag molecules, Applications. Conductometric sensors, Coulometric sensors, Voltammetric sensors, Applications, Neurotransmitters, Amperometric sensors, Chronoamperometric analysis, Multichannel sensors, Microelectrode sensors, Electrochemical Impedance Sensors, Quartz crystal nanobalance sensors, Molecular recognition, Applications. Surface Plasmon resonance based sensors, Fiber optic sensors, Twodimensional microarray based sensors, Applications for Food Safety - Mycotoxins, adultrants, Biomedical diagnosis - Cancer markers.

Books suggested:

1. Molecular mechanics. By U.Bukert and N.L.Allinger, ACS Monograph 177,1982
2. Organic Chemistry book of Orbitals. L.Salem and W.L.Jorgenson
3. Mechanism and theory in Organic Chemistry, T.M.Lowry, K.C.Richardson, Harper and Row
4. Introduction to theoretical Organic Chemistry and molecular modeling by W.B.Smith, VCH, Weinheim.
5. Physical Organic chemistry, N.S.Isaac
6. Supramolecular Chemistry - concepts and perspectives by J M .Lehn,
7. The Physical basis of Organic Chemistry by H.Maskill.
8. Physical Organic Chemistry by Jack Hine Laboratory course
9. Brian R. Egdins, Chemical Sensors and Biosensors, Analytical Techniques in the Sciences (ANTS), 2nd Edition, Wiley, 2002.
10. Gabor Harsanyi, Sensors in Biomedical Applications - Fundamentals, Technology and Applications, CRC Press, 2000.
11. Raluca-Ioana Stefan, Electrochemical Sensors in Bioanalysis, CRC Press, 2001.

ELECTIVE –4A (ID PAPER)**PAPER III CH(PC)- 403T(CB3): MOLECULAR MODELING AND IT'S APPLICATIONS**

PC(CB3)-25: Molecular Modeling – I

PC(CB3)-26: Molecular Modeling – II

PC(CB3)-27: Drug Design Methods I - Ligand Based

PC(CB3)-28: Drug Design Methods II - Structure Based.

PC(CB3)-25: Molecular Modeling – I

(15hrs)

Introduction to Molecular Modeling, Single molecule calculations, assemblies of molecules and reactions of molecules - Co-ordinate systems; Cartesian and Internal Co-ordinates, Z-matrix - Potential energy surface - Conformational search; Global minimum, Local minimum, Conformational analysis of ethane.

Force field ; Features of Molecular Mechanics, Bonded and Non-bonded interactions, Bond Stretching, Angle Bending, Torsional Terms (Improper Torsions, out of Plane Bending Motions, Cross Terms), Non Bonded Interactions (Electrostatic Interactions, Van-der Waals interactions), Hydrogen Bonding Interactions.

PC(CB3)-26: Molecular Modeling – II

(15hrs)

Force Field Equation in Energy minimization (Energy as function of r , θ , ω) - Introduction to Derivative Minimization Methods (First Order Minimization), Types of energy minimization Methods ; Steepest Descent, Conjugate Gradient, Conformational Search procedures - Geometry optimization procedures - Molecular Dynamics: Introduction, description of Molecular Dynamics, basic elements of Monte-Carlo method, differences between Molecular Dynamics and Monte-Carlo method, Qualitative exposure to Molecular Dynamics Simulations.

PC(CB3)-27: Drug Design Methods I - Ligand Based

(15hrs)

Lead Molecule - Structure Activity Relationship (SAR), Quantitative Structure Activity Relationship (QSAR), Distinguish between SAR and QSAR - Physicochemical parameters ; Electronic effects, Hydrophobicity, Steric Factors Taft's Steric function, Molar Refractivity, Verloop Steric factor - Molecular Descriptor analysis: Craig plot, Topliss scheme, Bioisosteres - Hansch model, Free-Wilson model for QSAR equations - Regression analysis: Multi Linear Regression and Partial Least Square (terms: n, SD, r, r², r²%, F) - Examples for linear and non-linear equations - 3D QSAR: CoMFA and CoMSIA - Differences between 2D and 3D QSAR.

PC(CB3)-28: Drug Design Methods II - Structure Based.

(15hrs)

Database similarity searches - Pair-wise alignment: Global sequence analysis (Needleman-Wunsch), Local Sequence Alignment (Smith Waterman), Multiple Sequence Alignment - Homology Modeling: Query sequence, Template selection, Alignment, Backbone Modeling, Loop Modeling, Side chain Modeling, Model optimization, Energy minimization - Model Evaluation: Ramachandran Plot, Verify 3D, Errata and ProSA - Active site Identification - Docking, Docking Algorithms: Genetic Algorithm, Incremental construction - Molecular Interactions, Scoring functions - Virtual Screening: Ligand Based and Structure Based. De novo ligand design and its limitations.

Books suggested:

1. Molecular Modelling: Principles and Applications, by Andrew Leach, Longman Publications.
2. Computational Chemistry, Guy H. Grant & W. Graham Richards, Oxford University Press.
3. Computational Chemistry: Introduction to the theory and Applications of Molecular and Quantum Mechanics, Errol Lewars, Springer Publications.
4. Recent advances in Bioinformatics by I. A. Khan and A Khanum Ukaaz publications, 2003.
5. Molecular modelling – Basic Principles and Applications by Hans Dieter Holtje and Gerd Folkers, Wiley-VCH, 1996
6. Introduction to Computational Chemistry by Jensen, Wiley Publishers, second edition
7. Bioinformatics – A Primer by P. Narayanan, New Age International, (PC) Ltd, 2005.
8. Introduction to Bioinformatics by Arthur M. Lesk, Oxford University Press (Indian. Edition), 2002
9. Principles of Medicinal Chemistry Vol. II by Dr. SS Kadam Pragati books Pvt. Ltd; 2007
10. An Introduction to Medicinal Chemistry by G L Patrick, Oxford University Press
11. Bioinformatics: Methods and Applications: Genomics, Proteomics and Drug Discovery. S.C. Rastog, Namita Mendiratta, Parag Rastogi, PHI Larning Pvt. Ltd; 2006
12. Pharmacy Practice Vol.I and II by Remington, Pharmaceutical Press
13. Burger's Medicinal Chemistry and Drug Discovery, 5th Edition, Wiley-Interscience, New York
14. Text book of Drug design and Vol.1 discovery 3rd Edition by POVL krogsgaard- Larsen Tommy liljefors and ULF Madsen.

ELECTIVE –4B (ID PAPER)**PAPER-IV CH(PC) 404T(CB4): Engineering Chemistry**

PC(CB4) -29: Water And Waste Water Treatment

PC(CB4) -30: Corrosion And Its Control

PC(CB4) -31: Energy Sources

PC(CB4)- 32 Engineering Materials

PC(CB4) -29:Water and waste water treatment (15 hrs)

Review of Hardness: causes, measurement of hardness, units- types of hardness, estimation of temporary and permanent hardness, numerical problems. Boiler troubles- scales and sludge formation, caustic embrittlement, priming and foaming. Methods for boiler water treatment: Soda-lime process, zeolite process, ion exchange process. Treating saline water: distillation, electro dialysis, reverse osmosis. Municipal water supply: sedimentation, filtration, sterilization. Waste water treatment: physical, chemical and biological treatment. Sewage water , COD and BOD , numerical problems

PC(CB4) -30:Corrosion and its control: (15 hrs)

Magnitude of the problem, theories of corrosion, Chemical and electrochemical corrosion, corrosion reactions, factors affecting corrosion- nature of metal, purity of metal,electrochemical series, over voltage, nature of oxide film, nature of corrosion product, nature of environment, effect of temperature, effect of pH, effect of oxidant, humidity. Corrosion control methods- design and material selection, cathodic protection, sacrificial anode, impressed current cathode. Surface coating methods: Surface preparation, metallic coatings, application of metal coatings: hot dipping, galvanizing, tinning, cladding, electroplating, chemical conversion coatings. Organic surface coatings-paints, constituents of paints and their functions, methods of application of paints, failure of paint films, varnishes, enamels, lacquers.

PC(CB4) -31: Energy sources: (15 hrs)

Conventional energy resources: Chemical fuels, classification, (solids, liquids, gaseous) . Solid fuels: coal, analysis of coal , proximate and ultimate analysis and their significance. Liquid fuels: petroleum, refining of petroleum, cracking, reforming. Synthetic petrol - Bergius and Fischer-Tropsch's process, knocking, anti knocking agents, octane number. Diesel fuel: Cetane number. Other liquid fuels: LPG, biodiesel, kerosene, fuel oil, benzol, tar, power alcohol. Gaseous fuels: natural gas, coal gas, producer gas, oil gas, water gas, biogas, Combustion: Calorific value and its determination, bomb calorimeter. HCV and LCV values of fuels, problems. analysis of flue gas by Orsats method. Rocket fuels, solid propellants, liquid propellants, monopropellants, bipropellants.

Non conventional energy resources: Nuclear fuels- nuclear reactor, nuclear fission, nuclear fusion, sources of nuclear fuels, disposal of radio active wastes, reprocessing of nuclear fuels. solar, hydro, wind, tidal energies. Bio fuels, H₂ as a non polluting fuel.

PC(CB4) -32: Engineering materials.

(15 hrs)

Cement: composition of Portland cement, analysis, setting and hardening of Portland cement (reactions), decay of cement concrete, lime, manufacture, types of lime, plaster of paris

Lubricants: Criterion of a good lubricant, classification of lubricants: petroleum oils, fixed oils, synthetic lubricants, semisolid lubricants, solid lubricants. Properties of lubricants: cloud point, pour point, flash and fire point, viscosity.

Refractories: Classification, characteristics of good refractory, failure of refractories. Glass, glass making oxides and their functions, manufacture of glass. Porcelain, enamels, abrasives.

Conductors and insulators: Classification of insulators, characteristics of thermal and electrical insulators and super conductors (Nb-Sn alloy, $YBa_2Cu_3O_{7-x}$) applications.

Composite materials: Advantageous properties of the composites, classification, mechanism of strengthening, mechanism of hardening of particle reinforcement, fabrication of the composites.

Liquid crystals: Characteristics of liquid crystal orders, physical properties of liquid crystals, classification of Liquid crystals, types of mesophases chemical nature of Liquid crystals, applications of Liquid crystals, future of liquid crystals.

Books suggested:

1. Text book of Engineering Chemistry by C.P. Murthy, C.V. Agarwal & A. Naidu: B.S. Publications, Hyderabad (2006).
2. Text book of Engineering Chemistry by S.S. Dara: S. Chand & Co. New Delhi (2006).
3. Engineering Chemistry by B. Siva Shanker : Mc-Graw Hill publishing Company Limited, New Delhi (2006)
4. Engineering Chemistry by J.C. Kuriocose & J. Rajaram, Tata McGraw Hill Co. New Delhi (2004)
5. Engineering Chemistry by P.C. Jain & Monica Jain, Dhanpatrai publishing company, (2008)
6. Chemistry of Engineering Materials by C.V. Agarwal, C.P. Murthy & A. Naidu: BS publications
7. Chemistry of Engineering Materials by R.P. Mani & K.N. Mishra, CENGAGE learning
8. Applied Chemistry – A text book of engineering and Technology – Springar (2005)
9. Text book of Engineering Chemistry by Shasi Chawla: Dhanpatrai Publishing company, New Delhi (2008)
10. Engineering Chemistry by R. Gopalan, D. Venkatappayya & D.V. Sulochana Nagarajan – Vikas Publishers (2008).

ELECTIVE-4C (ID PAPER)**PAPER-IV CH(PC) 404T(CB5): Sugar Chemistry AND Sugar Technology**

PC(CB5) -33: Advanced Sugar Chemistry

PC(CB5) -34: Sugar & Sugar byproducts

PC(CB5) -35: Methodology used in Sugar Analysis

PC(CB5)- 36: Sugar Technology and Management

PC(CB5) -33: Advanced Sugar Chemistry: (15 hrs)

Carbohydrate nomenclature. Fischer, Haworth and conformational structures of mono and oligo saccharides. Chemical reactivity of sugars. Reducing and non-reducing sugars. Chiral nature of sugars. R-S nomenclature, Fischer D-L nomenclature of sugars. Sugar enantiomers, diastereo isomers, epimers and enomers. Acyclic structure of sugars, determination of relative and absolute configuration of sugars. Cyclic forms of sugars. Conformational analysis of sugars. Hassel- Otter effect. Delta-two effect. Anomeric effect. Calculation of conformational free energies. Optical rotation, specific rotation and molecular rotation of sugars. General epimer rule. Relationship between rotation and conformation. Stereo chemical transformations. Mutarotation, enolization, isomerization, anhydride formation and reversion, pH stability of glucose and fructose, protection of sugar hydroxyls.

PC(CB5) -34: Sugar & Sugar byproducts: (15 hrs)

Structure determination of sucrose, synthesis of sucrose, biosynthesis of sucrose, chemical nature of sucrose. Oligo saccharide synthesis. Oligo saccharide optical rotating power (Hudson and Klyn rules). ¹³C NMR spectroscopic data of glucose, fructose and sucrose. Uses of sugar chirons in organic synthesis. Sugar byproducts. Bagasse, molasses and press mud. Bagasse- characteristics and uses. Production of biogas, fiberboard and furfural. Press mud- extraction of cane wax, press mud and manure. Molasses- fermentation of molasses. Production of alcohol and rectified spirit.

PC(CB5) -35: Methodology used in Sugar Analysis: (15 hrs)

Sampling techniques. Determination of moisture in bagasse, molasses and cane sugar. Methods of estimation of total soluble solids in sugar and sugar house products. Optical methods of sugar analysis, sugar scales and normal weight. Estimation of reducing sugars and sugar present in cane juice by Eynon & Lane, Luff & Schoorl and Benedicts methods. Determination of sugars by Invertase method, Jackson- Gellis, Munsen- Walker's Cu₂O and De Whalleys' volumetric method. Determination of Ash by Carbonate- Ash and Cuitometric (Conductometric) methods. Determination of various other constituents present in raw sugars. Estimation and chemical composition of cane and its juice.

Instrumental methods of sugar industry- Static characteristics and Dynamic characteristics. Gas, liquid, vapor thermometers. Bimetallic thermometers and thermocouples. Electronic panometer, cuitometer. Introduction to pneumatic control systems and elements. Working principle and instrumentation methodology of potentiometer, pH meter, polarimeter and cuitometer.

PC(CB5) -36: Sugar Technology and Basic Principles of Management: (15 hrs)

Sugar Technology: Cane juice interaction, maceration and imbibition. Principles of cane juice clarification, defecation and sulphitation. Juice heaters, filters and reaprovation vaccum pans. Centrifuges. Sugar driers and molasses. Introductory treatment of chemical control (i) Milling Control and (ii) Boiling house control.

Management: Concept and philosophy of management in major and small-scale industries. Location of factory site and Lay out of plant. Joint stock companies. Co-operative Societies. Production management and control. Personnel administration, purchases and sales, organization and control.

Books suggested:

1. Cane Sugar Hand Book, Maede & Chen, John Wiely & Sons
2. Determination of Food Carbohydrates, D. A. T. Southgate, Applied Science Publishers, London
3. Text Book of Sugar Chemistry and Sugar Technology, Mathur
4. Text Book of Sugar Byproducts, Morris Patrov
5. A Hand Book of Qualitative and Quantitative Organic Analysis, H. J. Clark, Orient Longman
6. Text Book of Biochemistry, Lehninger
7. Analysis of Sugars, Pleus
8. Text Book of Sugar Technology, Hugot
9. Instrumental Methods in Sugar Industry, Eckman
10. Principles of Instrumental Analysis, Skoog and West
11. Technical Methods of Analysis, Griffith, McGraw Hill
12. Advanced Sugar Chemistry, R. S. Shellaxberges
13. Sugar, John Yulkin, Jack Edelman, Liesel Hough
14. International Uniform Methods for Sugar Analysis, H. C. S. De Whelly

IV SEMESTER PRACTICALS

Note: The data obtained in all the experiments are to be analyzed by the students both *by the usual graphical methods and by regression (linear/nonlinear) techniques using a PC.*

CH (PC) 451P: Paper-V (Chemical Kinetics)

9hrs/week

◆ **Study of acetone-iodine reaction by spectrophotometry**

1. Order w.r.t. [iodine]
2. Order w.r.t. [acetone]
3. Order w.r.t. [H⁺]

◆ **Study of peroxydisulphate – iodide reaction by colorimetry**

◆ **Study of saponification of ethyl acetate by conductometry:**

1. Overall order of the reaction
2. Order w.r.t. [ethyl acetate]
3. Order w.r.t. [NaOH]

◆ **Study of solvolysis of t-butylchloride by conductometry:**

effect of solvent dielectric constant/
polarizability (methanol/water mixture) on the rate of solvolysis

◆ **Study of oxidation of primary alcohols by dichromate by spectrophotometry:**

Application of Taft equation

CH (PC) 452P: Paper-VI (Instrumentation)

9 hrs/week

Spectrophotometry:

- ◆ Estimation of Cu(II) using EDTA
- ◆ Estimation of Fe(III) using thiocyanate
- ◆ Estimation of Fe(II) using 1,10-phenanthroline
- ◆ Estimation of Fe(III) in tap water using thiocyanate by standard addition method
- ◆ Simultaneous determination of dichromate and permanganate in a mixture
- ◆ Spectrophotometric titrations: Cu(II) vs EDTA
Fe(II) vs 1,10-phenanthroline
- ◆ Composition of Cu(II) – EDTA complex by Job's method
- ◆ Composition of Fe(II) – phenanthroline complex – Job's method, mole ratio, slope ratio method.
- ◆ Determination of composition and Gibbs energy of formation of Fe(III)–salicylic acid complex
- ◆ Determination of pK_a of methyl red indicator
- ◆ Estimation of Mn(II) by spectrophotometry using periodate.

Potentiometry:

- ◆ Potentiometric titrations:
 1. Weak acids vs strong base and calculation of dissociation constants
 2. Mixture of strong and weak acids vs strong base
 3. Dibasic acid vs strong base
 4. Fe(II) vs Ce(IV) and calculation of formal redox potential of Fe(II)/Fe(III)
 - ◆ Fe(II) vs MnO₄⁻
 - ◆ Fe(III) vs EDTA
 - ◆ Mixture of halides vs AgNO₃
 - ◆ Mixture of KI and KSCN vs AgNO₃

Polarography:

- ◆ Estimation of Pb²⁺, Cd²⁺ and Ni²⁺ separately and in a mixture.

Suggested books:

1. A textbook of practical organic chemistry by A I Vogel, Vol 1&2.
2. Senior practical physical chemistry. B. D. Khosla, V.C. Garg, Adarsh Gulati
3. Experimental Physical Chemistry: V. Athawale and P. Mathur.
4. Practical Physical Chemistry: B. Vishwanathan and P.S. Raghavan.
5. Practical in Physical Chemistry: P.S. Sindhu
6. Advanced Practical Physical chemistry: J.B. Yadav