Structure and Detailed Syllabus of the Undergraduate Course (B.Sc.) in Chemistry under CBCS

Department of Chemistry

Presidency University

PRESIDENCY UNIVERSITY
KOLKATA

Department of Chemistry
(Faculty of Natural and Mathematical Sciences)
Presidency University
Hindoo College (1817-1855), Presidency College (1855-2010)
86/1, College Street, Kolkata - 700 073
West Bengal, India

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Structure of Chemistry Courses

Semester	Number of Course			
	Core Course	SEC (out of)	DSE (out of)	GE (out of)
1^{st}	2	-	-	1
2^{nd}	2	-	-	1
3^{rd}	3	1 (3)	-	1 (2)
4^{th}	3	1 (3)	-	1 (2)
5^{th}	2	-	2 (6)	-
6^{th}	2	-	2 (7)	-
Total	**14**	**2**	**4**	**4**

Credit Allocation and Marks Distribution for the Undergraduate Course in Chemistry (Major) under CBCS
Department of Chemistry, Presidency University, Kolkata

Semester	Course Type	Paper Code	Course Name	Marks					
				Theory	Practical	Total	Theory	Practical	Total
First	Core Course	CHEM01C1	INORGANIC CHEMISTRY-I	4	2	6	70	30	**100**
First	Core Course	CHEM01C2	PHYSICAL CHEMISTRY-I	4	2	6	70	30	**100**
First	Generic Elective	CHEM01GE1	Atomic Structure, Bonding, General Organic Chemistry, Aliphatic Hydrocarbons	4	2	6	70	30	**100**
First	Ability Enhancement Compulsory Course	AECC01	Environmental Science / English Communication	4		4	100		**100**
Second	Core Course	CHEM02C3	ORGANIC CHEMISTRY-I	4	2	6	70	30	**100**
Second	Core Course	CHEM02C4	PHYSICAL CHEMISTRY-II	4	2	6	70	30	**100**
Second	Generic Elective	CHEM02GE2	Chemical Energetics, Equilibria and Functional Organic Chemistry	4	2	6	70	30	**100**
Second	Ability Enhancement Compulsory Course	AECC02	Environmental Science / English Communication	4		4	100		**100**
Third	Core Course	CHEM03C5	INORGANIC CHEMISTRY-II	4	2	6	70	30	**100**
Third	Core Course	CHEM03C6	ORGANIC CHEMISTRY-II	4	2	6	70	30	**100**
Third	Core Course	CHEM03C7	PHYSICAL CHEMISTRY-III	4	2	6	70	30	**100**
Third	Generic Elective	CHEM03GE3.1 CHEM03GE3.2	1.Solutions, Phase Equilibria, Conductance, Electrochemistry & Functional Group Organic Chemistry *OR* 2.Molecules of Life	4	2	6	70	30	**100**
Third	Skill Enhancement Course	CHEM03SEC1.1 CHEM03SEC1.2	1.IT Skills for Chemists *OR* 2.Basic Analytical and Nuclear Chemistry	4		4	100		**100**
Fourth	Core Course	CHEM04C8	INORGANIC CHEMISTRY-III	4	2	6	70	30	**100**
Fourth	Core Course	CHEM04C9	ORGANIC CHEMISTRY-III	4	2	6	70	30	**100**
Fourth	Core Course	CHEM04C10	PHYSICAL CHEMISTRY-IV	4	2	6	70	30	**100**
Fourth	Generic Elective	CHEM04GE4.1 CHEM04GE4.2	1.Transition Metal & Coordination Chemistry, States of Matter & Chemical Kinetics *OR* 2.Quantum Chemistry, Spectroscopy & Photochemistry	4	2	6	70	30	**100**
Fourth	Skill Enhancement Course	CHEM04SEC2.1 CHEM04SEC2.2	1.Green Methods in Chemistry *OR* 2.Pharmaceutical Chemistry	4		4	100		**100**
Fifth	Core Course	CHEM05C11	ORGANIC CHEMISTRY-IV	4	2	6	70	30	**100**
Fifth	Core Course	CHEM05C12	PHYSICAL CHEMISTRY-V	4	2	6	70	30	**100**
Fifth	Discipline Specific Elective	CHEM05DSE1.*	Discipline Specific Elective*	4	2	6	70	30	**100**
Fifth	Discipline Specific Elective	CHEM05DSE2.*	Discipline Specific Elective*	4	2	6	70	30	**100**
Sixth	Core Course	CHEM06C13	INORGANIC CHEMISTRY-IV	4	2	6	70	30	**100**
Sixth	Core Course	CHEM06C14	ORGANIC CHEMISTRY-V	4	2	6	70	30	**100**
Sixth	Discipline Specific Elective	CHEM06DSE3.**	Discipline Specific Elective**	4	2	6	70	30	**100**
Sixth	Discipline Specific Elective	CHEM06DSE4.**	Discipline Specific Elective**	4	2	6	70	30	**100**
			Total:	104	44	**148**	1940	660	**2600**

*** 1. Applications of Computers in Chemistry, 2. Polymer Chemistry, 3. Analytical Methods in Chemistry,** 4. Research Methodology for Chemistry, 5. Molecular Modelling & Drug Design, 6. Industrial Chemicals & Environment. **** 7. Fluorescence study for the sensing and macromolecular interactions, 8. Seminar / Review / Grand Viva, 9. Retrosynthesis and strategy for organic synthesis,** 10. Inorganic Materials of Industrial Importance, 11. Green Chemistry, 12. Instrumental Methods of Analysis, 13. Novel Inorganic Solids

Semester-wise Modules of the Undergraduate Course in Chemistry (Major) under CBCS Department of Chemistry, Presidency University, Kolkata

Semester I

CHEM01C1	INORGANIC CHEMISTRY-I
CHEM01C2	PHYSICAL CHEMISTRY-I
CHEM01GE1	Generic Elective-I

Semester II

CHEM02C3	ORGANIC CHEMISTRY-I
CHEM02C4	PHYSICAL CHEMISTRY-II
CHEM02GE2	Generic Elective-II

Semester III

CHEM03C5	INORGANIC CHEMISTRY-II
CHEM03C6	ORGANIC CHEMISTRY-II
CHEM03C7	PHYSICAL CHEMISTRY-III
CHEM03GE3	Generic Elective-III
CHEM03SEC1	Skill Enhancement Course-I

Semester IV

CHEM04C8	INORGANIC CHEMISTRY-III
CHEM04C9	ORGANIC CHEMISTRY-III
CHEM04C10	PHYSICAL CHEMISTRY-IV
CHEM04GE4	Generic Elective-IV
CHEM04SEC2	Skill Enhancement Course-II

Semester V

CHEM05C11	ORGANIC CHEMISTRY-IV
CHEM05C12	PHYSICAL CHEMISTRY-V
CHEM05DSE1	Discipline Specific Elective-I
CHEM05DSE2	Discipline Specific Elective-II

Semester VI

CHEM06C13	INORGANIC CHEMISTRY-IV
CHEM06C14	ORGANIC CHEMISTRY-V
CHEM06DSE3	Discipline Specific Elective-III
CHEM06DSE4	Discipline Specific Elective-IV

Academic Session: Each Semester shall contain at least 16 Teaching Weeks

Odd Semesters: Semesters One, Three and Five - July to December
Even Semesters: Semesters Two, Four and six - January to June

CORE COURSE (HONOURS IN CHEMISTRY)

Semester I:

1. CHEMISTRY-C1: INORGANIC CHEMISTRY-I (Credits: Theory-04, 60 Lectures), CHEMISTRY PRACTICAL- C1 LAB: (Credits: Practicals-02, 60 Lectures)

2. CHEMISTRY-C2: PHYSICAL CHEMISTRY-I (Credits: Theory-04, 60 Lectures), CHEMISTRY PRACTICAL – C2 LAB: (Credits: Practicals-02, 60 Lectures)

Semester II:

3. CHEMISTRY-C3: ORGANIC CHEMISTRY-I (Credits: Theory-04, 60 Lectures), CHEMISTRY PRACTICAL – C3 LAB: (Credits: Practicals-02, 60 Lectures)

4. CHEMISTRY-C4: PHYSICAL CHEMISTRY-II (Credits: Theory-04, 60 Lectures), CHEMISTRY PRACTICAL – C4 LAB: (Credits: Practicals-02, 60 Lectures)

Semester III:

5. CHEMISTRY-C5: INORGANIC CHEMISTRY-II (Credits: Theory-04, 60 Lectures), CHEMISTRY PRACTICAL – C5 LAB: (Credits: Practicals-02, 60 Lectures)

6. CHEMISTRY-C6: ORGANIC CHEMISTRY-II (Credits: Theory-04, 60 Lectures), CHEMISTRY PRACTICAL – C6 LAB: (Credits: Practicals-02, 60 Lectures)

7. CHEMISTRY-C7: PHYSICAL CHEMISTRY-III (Credits: Theory-04, 60 Lectures), CHEMISTRY PRACTICAL – C7 LAB: (Credits: Practicals-02, 60 Lectures)

Semester IV:

8. CHEMISTRY-C8: INORGANIC CHEMISTRY-III (Credits: Theory-04, 60 Lectures), CHEMISTRY PRACTICAL – C8 LAB: (Credits: Practicals-02, 60 Lectures)

9. CHEMISTRY-C9: ORGANIC CHEMISTRY-III (Credits: Theory-04, 60 Lectures), CHEMISTRY PRACTICAL – C9 LAB: (Credits: Practicals-02, 60 Lectures)

10. CHEMISTRY-C10: PHYSICAL CHEMISTRY-IV (Credits: Theory-04, 60 Lectures),

CHEMISTRY PRACTICAL – C10 LAB: (Credits: Practicals-02, 60 Lectures)

Semester V:

11. CHEMISTRY-C11: ORGANIC CHEMISTRY-IV (Credits: Theory-04, 60 Lectures), CHEMISTRY PRACTICAL – C11 LAB: (Credits: Practicals-02, 60 Lectures)

12. CHEMISTRY-C12: PHYSICAL CHEMISTRY-V (Credits: Theory-04, 60 Lectures), CHEMISTRY PRACTICAL - C12 LAB: (Credits: Practicals-02, 60 Lectures)

Semester VI:

13. CHEMISTRY-C13: INORGANIC CHEMISTRY-IV (Credits: Theory-04,60 Lectures), CHEMISTRY PRACTICAL – C13 LAB: (Credits: Practicals-02, 60 Lectures)

14. CHEMISTRY-C14: ORGANIC CHEMISTRY-V (Credits: Theory-04, 60 Lectures), CHEMISTRY PRACTICAL – C14 LAB: (Credits: Practicals-02, 60 Lectures)

CHEMISTRY-DSE (ELECTIVES)

Credit: 4 + 2

Semester V:

1. Applications of Computers in Chemistry (4) + Lab (4)

2. Polymer Chemistry (4) + Lab (4)

3. Analytical Methods in Chemistry (4) + Lab (4)

4. Research Methodology for Chemistry (5) + Tutorials (1)

5. Molecular Modelling & Drug Design (4) + Lab (4)

6. Industrial Chemicals & Environment (4) + Lab (4)

Semester VI:

7. Fluorescence study for the sensing and macromolecular interactions (4) + Lab (4)

8. Seminar / Review / Grand Viva

9. Retrosynthesis and strategy for organic synthesis (4) + Lab (4)

10. Inorganic Materials of Industrial Importance (4) + Lab (4)

11. Green Chemistry (4) + Lab (4)

12. Instrumental Methods of Analysis (4) + Lab (4)

13. Novel Inorganic Solids (4) + Lab (4)

SKILL ENHANCEMENT COURSES (SEC)

Credit: 4

Semester III:

1. IT Skills for Chemists
2. Basic Analytical and Nuclear Chemistry

Semester IV:

3. Green Methods in Chemistry
4. Pharmaceutical Chemistry

GENERIC ELECTIVE PAPERS (GE) MINOR CHEMISTRY

Credit: 4+2

Semester I:

1. Atomic Structure, Bonding, General Organic Chemistry, Aliphatic Hydrocarbons (4 + 4)

Semester II:

2. Chemical Energetics, Equilibria and Functional Organic Chemistry (4 + 4)

Semester III:

3. Solutions, Phase Equilibria, Conductance, Electrochemistry & Functional Group Organic Chemistry (4 + 4)

OR

Molecules of Life (4 + 4)

Semester IV:

4. Transition Metal & Coordination Chemistry, States of Matter & Chemical Kinetics (4+ 4)

OR

Quantum Chemistry, Spectroscopy & Photochemistry (4+4)

Semester I

CHEM01C1: INORGANIC CHEMISTRY-I

(Credits: Theory-04, 60 Lectures, Full Marks: 70)

Atomic Structure:

Bohr's theory, its limitations and atomic spectrum of hydrogen atom. Sommerfield modification. Wave mechanics: de Broglie equation, Heisenberg's Uncertainty Principle and its significance, Schrödinger's wave equation. Hydrogenic wavefunctions, Quantum numbers, introduction to the concept of atomic orbitals; shapes, radial and angular probability diagrams of s, p and d orbitals (qualitative idea). Many electron atoms and ions: Pauli's exclusion principle, Hund's rule, exchange energy, Aufbau principle and its limitations. Term symbols of atoms and ions. **(14 Lectures)**

Periodicity of Elements:

s, *p*, *d*, *f* block elements, the long form of periodic table. Detailed discussion of the following properties of the elements, with reference to *s* and *p*-block – group trend and periodic trend.

(a) Effective nuclear charge, shielding or screening effect, Slater rules, variation of effective nuclear charge in periodic table.

(b) Atomic radii (van der Waals)

(c) Ionic and crystal radii.

(d) Covalent radii (octahedral and tetrahedral)

(e) Ionization enthalpy, Successive ionization enthalpies and factors affecting ionization energy. Applications of ionization enthalpy.

(f) Electron gain enthalpy, trends of electron gain enthalpy.

(g) Electronegativity, Pauling's/ Mulliken's/ Allred Rachow's/ and Mulliken-Jaffé's electronegativity scales. Variation of electronegativity with bond order, partial charge, hybridization, group electronegativity.

(16 Lectures)

Chemical Bonding:

(i) *Ionic bond:* General characteristics, types of ions, size effects, radius ratio rule and its limitations. Packing of ions in crystals. Born-Landé equation with derivation and importance of Kapustinskii expression for lattice energy. Madelung constant, Born-Haber cycle and its application, Solvation energy.

(ii) *Covalent bond:* Lewis structure, Valence Bond theory (Heitler-London approach). Hybridization, equivalent and non-equivalent hybrid orbitals. Bent's rule, Resonance and resonance energy, Molecular orbital theory. Molecular orbital diagrams of diatomic and simple polyatomic molecules N_2, O_2, C_2, B_2, F_2, CO, NO, HCl,

BeF_2, CO_2, (idea of s-p mixing and orbital interaction to be given). Formal charge, Valence shell electron pair repulsion theory (VSEPR), shapes of simple molecules and ions containing lone pairs and bond pairs of electrons, multiple bonding (σ and π bond approach) and bond lengths.

Covalent character in ionic compounds, polarizing power and polarizability. Fajan's rule and consequences of polarization.

Ionic character in covalent compounds: Bond moment and dipole moment. Percentage ionic character from dipole moment and electronegativity difference.

(iii) *Metallic Bond:* Qualitative idea of valence bond and band theories. Semiconductors and insulators, defects in solids.

(iv)*Weak Chemical Forces:* van der Waals forces, ion-dipole forces, dipole-dipole interactions, induced dipole interactions, Instantaneous dipole-induced dipole interactions. Repulsive forces, Hydrogen bonding (theories of hydrogen bonding, valence bond treatment) Effects of chemical force, melting and boiling points.

(20 Lectures)

Oxidation-Reduction:

Elementary idea on standard redox potentials with sign convention, Nernst equation. Influence of complex formation, precipitation and change of pH on redox potentials, formal potential. Feasibility of a redox titration, redox potential at the equivalence point, redox indicators, redox potential diagram (Latimer and Frost) of common elements and their applications. Disproportionation and comproportionation reactions (typical examples). **(10 Lectures)**

Reference Books:

- Lee, J.D. Concise Inorganic Chemistry ELBS, 1991.
- Douglas, B.E. and McDaniel, D.H. Concepts & Models of Inorganic Chemistry Oxford, 1970
- Atkins, P.W. & Paula, J. Physical Chemistry, 10th Ed., Oxford University Press, 2014.
- Day, M.C. and Selbin, J. Theoretical Inorganic Chemistry, ACS Publications, 1962.
- Rodger, G.E. Inorganic and Solid State Chemistry, Cengage Learning India Edition, 2002.

CHEMISTRY PRACTICAL- C1 LAB:

(Credits: Practicals-02, 60 Lectures, Full marks: 30)

Elementary idea of redox titration using $KMnO_4$ and $K_2Cr_2O_7$ (theory)

(A) Titrimetric Analysis

(i) Calibration and use of apparatus

(ii) Preparation of solutions of different Molarity/Normality of titrants

(B) Acid-Base Titrations

(i) Estimation of carbonate and hydroxide present together in mixture.

(ii) Estimation of carbonate and bicarbonate present together in a mixture.

(iii) Estimation of free alkali present in different soaps/detergents

(C) Oxidation-Reduction Titrimetry

(i) Estimation of Fe(II) and oxalic acid using standardized $KMnO_4$ solution.

(ii) Estimation of oxalic acid and sodium oxalate in a given mixture.

(iii) Estimation of Fe(II) with $K_2Cr_2O_7$.

Reference Book:

1. Mendham, J., A. I. Vogel's Quantitative Chemical Analysis 6th Ed., Pearson, 2009.

CHEM01C2: PHYSICAL CHEMISTRY-I

(Credits: Theory-04, 60 Lectures, Full Marks: 70)

Gaseous state: Kinetic molecular model of a gas: postulates and derivation of the kinetic gas equation; The Barometric distribution law; Maxwell distribution and its use in evaluating molecular velocities (average, root mean square and most probable) and average kinetic energy, idea about gamma function and related integral, error function, Maxwell distribution for kinetic energy, Maxwell –Boltzman distribution law; law of equipartition of energy, degrees of freedom and molecular basis of heat capacities.

Collision frequency; collision diameter; mean free path and viscosity of gases, including their temperature and pressure dependence, relation between mean free path and coefficient of viscosity, calculation of σ from η; variation of viscosity with temperature and pressure. Kinetic theory of gas in interpreting Fick's law of diffusion and Fourier law of heat conduction.

Behaviour of real gases: Deviations from ideal gas behaviour, Andrew's and Amagat's plots); compressibility factor, *Z*, and its variation with pressure for different gases. Causes of deviation from ideal behaviour. Van der Waals equation of state, its derivation and application in explaining real gas behaviour, mention of other equations of state (Berthelot, Dietrici); virial equation of state; van der Waals equation expressed in virial form and calculation of Boyle temperature. Isotherms of real gases and their comparison with van der Waals isotherms, continuity of states, critical state, relation between critical constants and van der Waals constants, law of corresponding states;

Intermolecular forces and potentials (Keesom, Debye and London), estimation of van der Waals constants, Lennard-Jones potential. **(22 Lectures)**

Liquid state: Qualitative treatment of the structure of the liquid state; physical properties of liquids; vapour pressure. Surface tension, surface energy (thermodynamic treatment), excess pressure, capillary rise and measurement of surface tension, work of cohesion and adhesion, spreading of liquid over other surface, vapour pressure over curved surface, temperature dependence of surface tension. General features of fluid flow (streamline and turbulent flows, Reynold's number); nature of viscous drag for streamline motion, Newton's equation, viscosity coefficient, Poisuille equation (with derivation), coefficient of viscosity. Stokes' law and terminal velocity; experimental determination of viscosity coefficient of liquids. Stokes'-Einstein relation for diffusivity, Effect of addition of various solutes on surface tension and viscosity. Temperature variation of viscosity of liquids and comparison with that of gases. Qualitative discussion of structure of water (qualitative idea). **(12 Lectures)**

Solid state: Nature of the solid state, law of constancy of interfacial angles, law of rational indices, Miller indices, elementary ideas of symmetry, symmetry elements and symmetry operations, qualitative idea of point and space groups, seven crystal systems and fourteen Bravais lattices; X-ray diffraction, Bragg's law, a simple account of rotating crystal method and powder pattern method. Analysis of powder diffraction patterns of NaCl, CsCl and KCl.

Defects in crystals. Glasses and liquid crystals. **(12 Lectures)**

Ionic equilibria:

Strong, moderate and weak electrolytes, degree of ionization, factors affecting degree of ionization, ionization constant and ionic product of water. Ionization of weak acids and bases, pH scale; dissociation constants of mono-, di-and triprotic acids (exact treatment).

Salt hydrolysis-calculation of hydrolysis constant, degree of hydrolysis and pH for different salts. Buffer solutions; derivation of Henderson equation and its applications; buffer capacity, buffer range, buffer action and applications of buffers in analytical chemistry and biochemical processes in the human body.

Solubility and solubility product of sparingly soluble salts – applications of solubility product principle.

Qualitative treatment of acid – base titration curves (calculation of pH at various stages). Theory of acid–base indicators; selection of indicators and their limitations.

(14 Lectures)

Reference Books:

- Atkins, P. W. & Paula, J. de Atkin's Physical Chemistry 10th Ed., Oxford University Press (2014).
- Ball, D. W. Physical Chemistry Thomson Press, India (2007).
- Castellan, G. W. Physical Chemistry 4th Ed. Narosa (2004).
- Mortimer, R. G. Physical Chemistry 3rd Ed. Elsevier: NOIDA, UP (2009).
- Engel, T. & Reid, P. Physical Chemistry 3rd Ed. Pearson (2013).

CHEMISTRY PRACTICAL-C2 LAB

(Credits: Practicals-02, 60 Lectures, Full Marks: 30)

1. **Surface tension measurements.**

a. Determine the surface tension.

b. Study the variation of surface tension of detergent solutions with concentration.

2. **Viscosity measurement using Ostwald's viscometer**.

a. Determination of viscosity of aqueous solutions of (i) polymer (ii) ethanol and (iii) sugar at room temperature.

b. Study the variation of viscosity of sucrose solution with the concentration of solute.

3. Indexing of a given powder diffraction pattern of a cubic crystalline system.

4. pH metry

a. Study the effect on pH of addition of HCl/NaOH to solutions of acetic acid, sodium acetate and their mixtures.

b. Preparation of buffer solutions of different pH

i. Sodium acetate-acetic acid

ii. Ammonium chloride-ammonium hydroxide

c. pH metric titration of (i) strong acid vs. strong base, (ii) weak acid vs. strong base.

d. Determination of dissociation constant of a weak acid.

Reference Books

- Khosla, B. D.; Garg, V. C. & Gulati, A. Senior Practical Physical Chemistry, R. Chand & Co.: New Delhi (2011).
- Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. Experiments in Physical Chemistry 8th Ed.; McGraw-Hill: New York (2003).
- Halpern, A. M. & McBane, G. C. Experimental Physical Chemistry 3rd Ed.; W.H. Freeman & Co.: New York (2003).

CHEM01GE1

Theory: Atomic Structure, Bonding, General Organic Chemistry, Aliphatic Hydrocarbons

(Credits: 04, 60 Lectures, Full Marks: 70)

Section A: Inorganic Chemistry

Atomic Structure:

Extra-nuclear Structure of atoms Bohr's theory for hydrogen atom (simple mathematical treatment), atomic spectra of hydrogen, quantum numbers and their significance, Pauli's exclusion principle, Hund's rule, electronic configuration of many- electron atoms, Aufbau principle and its limitations.

Stability of half-filled and completely filled orbitals, concept of exchange energy. Relative energies of atomic orbitals, Anomalous electronic configurations.

(14 Lectures)

Chemical Bonding and Molecular Structure:

*Ionic bonding:*General characteristics of ionic compounds, sizes of ions, radius ratio rule and its limitation. Lattice energy, Born Haber cycle.

Covalent bonding: General characteristics of covalent compounds, valence-bond approach, hybridization involving s, p, d orbitals. Valence Shell Electron Pair Repulsion (VSEPR) concept, shapes of simple molecules and ions of main group elements, bond moment and dipole moment, partial ionic character of covalent bonds, Fajan's rules, hydrogen bonding and its effect on physical and chemical properties.

MO Approach: Rules for the LCAO method, bonding and antibonding MOs and their characteristics for s-s, s-p and p-p combinations of atomic orbitals, nonbonding combination of orbitals, MO treatment of homonuclear diatomic molecules of 1st and 2nd periods (including idea of s-p mixing) and heteronuclear diatomic molecules such as CO and NO. Comparison of VB and MO approaches. **(16 Lectures)**

Section B: Organic Chemistry

Fundamentals of Organic Chemistry

Physical Effects, Electronic Displacements: Inductive Effect, Electromeric Effect, Resonance and Hyperconjugation. Cleavage of Bonds: Homolysis and Heterolysis. Structure, shape and reactivity of organic molecules: Nucleophiles and electrophiles. Reactive Intermediates: Carbocations, Carbanions and free radicals. Strength of organic acids and bases: Comparative study with emphasis on factors affecting pK values. Aromaticity: Benzenoids and Hückel’s rule.

(8 Lectures)

Stereochemistry

Conformations with respect to ethane, butane and cyclohexane. Interconversion of Wedge Formula, Newmann, Sawhorse and Fischer representations. Concept of chirality (upto two carbon atoms). Configuration:

Geometrical and Optical isomerism; Enantiomerism, Diastereomerism and Meso compounds). Threo and erythro; D and L; *cis* - *trans* nomenclature; CIP Rules: *R/ S* (for upto 2 chiral carbon atoms) and *E / Z* Nomenclature (for upto two C=C systems).

(10 Lectures)

Aliphatic Hydrocarbons

Functional group approach for the following reactions (preparations & reactions) to be studied in context to their structure. **Alkanes**: (Upto 5 Carbons). Preparation: Catalytic hydrogenation, Wurtz reaction, Kolbe's synthesis, from Grignard reagent. Reactions: Free radical Substitution: Halogenation. **Alkenes**: (Upto 5 Carbons) Preparation: Elimination reactions: Dehydration of alkenes and dehydrohalogenation of alkyl halides (Saytzeff's rule); *cis* alkenes (catalytic hydrogenation) and *trans* alkenes (Birch reduction). Reactions: *cis*-addition (alk. $KMnO_4$) and *trans*-addition (bromine), Addition of HX (Markownikoff's and anti-Markownikoff's addition), Hydration, Ozonolysis, Oxymecuration-demercuration, Hydroboration-oxidation. **Alkynes**: (Upto 5 Carbons) Preparation: Acetylene from CaC_2 and conversion into higher alkynes; by dehalogenation of tetra halides and dehydrohalogenation of vicinal-dihalides. Reactions: formation of metal acetylides, addition of bromine and alkaline $KMnO_4$, ozonolysis and oxidation with hot alk. $KMnO_4$.

(12 Lectures)

Reference Books:

• Lee, J.D. *Concise Inorganic Chemistry* ELBS, 1991.
• Cotton, F.A., Wilkinson, G. & Gaus, P.L. *Basic Inorganic Chemistry*, 3rd ed., Wiley.
• Douglas, B.E., McDaniel, D.H. & Alexander, J.J. *Concepts and Models in Inorganic Chemistry*, John Wiley & Sons.
• Huheey, J.E., Keiter, E.A., Keiter, R.L. & Medhi, O.K. *Inorganic Chemistry: Principles of Structure and Reactivity*, Pearson Education India, 2006.
• Graham Solomon, T.W., Fryhle, C.B. & Dnyder, S.A. *Organic Chemistry*, John Wiley & Sons (2014).
• McMurry, J.E. *Fundamentals of Organic Chemistry*, 7th Ed. Cengage Learning India Edition, 2013.
• Sykes, P. *A Guidebook to Mechanism in Organic Chemistry*, Orient Longman, New Delhi (1988).
• Eliel, E.L. *Stereochemistry of Carbon Compounds*, Tata McGraw Hill education, 2000.
• Finar, I.L. *Organic Chemistry* (Vol. I & II), E.L.B.S.
• Morrison, R.T. & Boyd, R.N. *Organic Chemistry*, Pearson, 2010.
• Bahl, A. & Bahl, B.S. *Advanced Organic Chemistry*, S. Chand, 2010.

GE1-Lab: (Credits: 02, 60 Lectures, Full Marks: 30)

Section A: Inorganic Chemistry - Volumetric Analysis (any four)

1. Estimation of sodium carbonate and sodium hydrogen carbonate present in a mixture.
2. Estimation of oxalic acid by titration with $KMnO_4$.
3. Estimation of water of crystallization in Mohr's salt by titration with $KMnO_4$.
4. Estimation of Fe(II) ions by titration with $K_2Cr_2O_7$.

5. Estimation of Cu(II) ions iodometrically using $Na_2S_2O_3$.

Section B: Organic Chemistry

1. Detection of extra elements (N, S, Cl, Br, I) in organic compounds (containing upto two extra elements)

2. Separation of mixtures by Chromatography: Measurement of Rf value in each case (combination of two compounds to be given)

(a) Identify and separate the components of a given mixture of two amino acids (glycine, aspartic acid, glutamic acid, tyrosine or any other amino acid) by paper chromatography

(b) Identify and separate the sugars present in the given mixture by paper chromatography.

Reference Books:

• Svehla, G. *Vogel's Qualitative Inorganic Analysis*, Pearson Education, 2012.
• Mendham, J. *Vogel's Quantitative Chemical Analysis*, Pearson, 2009.
• Vogel, A.I., Tatchell, A.R., Furnis, B.S., Hannaford, A.J. & Smith, P.W.G., *Textbook of Practical Organic Chemistry*, Prentice-Hall, 5th edition, 1996.
• Mann, F.G. & Saunders, B.C. *Practical Organic Chemistry* Orient-Longman, 1960.

Semester II:

CHEM02C3: ORGANIC CHEMISTRY- I

(Credits: Theory-04, Theory: 60 Lectures, Full Marks: 70)

Basics of Organic Chemistry & Reaction Mechanism

Organic Compounds: Classification, and Nomenclature, Hybridization, Shapes of molecules, Influence of hybridization on bond properties.

Electronic Effects: Inductive, electromeric, resonance and mesomeric effects, hyperconjugation and their applications; Dipole moment; Organic acids, bases and their relative strengths.

Homolytic and Heterolytic fission with suitable examples. Reaction Mechanism: ionic, radical and pericyclic; representation of mechanistic steps using arrow formalism, formal charges.

Reactive intermediates: carbocations (carbenium and carbonium ions), carbanions, carbon radicals, carbenes, nitrenes - structure using orbital picture, electrophilic / nucleophilic reactivity, stability, generation and fate. Electrophiles and Nucleophiles; Nucleophlicity and basicity;

Introduction to types of organic reactions and their mechanism: Addition, Elimination and Substitution reactions. **(6 Lectures)**

Reaction thermodynamics

Free energy and equilibrium, enthalpy and entropy factor, intermolecular & intramolecular reactions. Application of thermodynamic principles in tautomeric equilibria (keto-enol tautomerism). Composition of the equilibrium in different systems such as simple carbonyl, 1,3- and 1,2- dicarbonyl systems, phenols and related system; substituent and solvent effect *etc*.

(6 Lectures)

Stereochemistry:

Fischer Projection, Newmann and Sawhorse Projection formulae and their interconversions; Geometrical isomerism: *cis–trans* and, *syn-anti* isomerism *E*/*Z* notations with C.I.P rules.

Optical Isomerism: Optical Activity, Specific Rotation, Chirality/Asymmetry, Enantiomers, Molecules with two or more chiral-centres, Distereoisomers, *meso*-structures, Racemic mixture and resolution. Relative and absolute configuration: D/L and *R*/*S* designations.

(12 Lectures)

Aromatic Hydrocarbons

Aromaticity: Hückel's rule, aromatic character of arenes, cyclic carbocations/carbanions and heterocyclic compounds with suitable examples. Electrophilic aromatic substitution: halogenation, nitration, sulphonation and Friedel-Craft's alkylation/acylation with their mechanism. Directing effects of the groups.

(12 Lectures)

Chemistry of Aliphatic Hydrocarbons

A. Carbon-Carbon sigma bonds

Chemistry of alkanes: Formation of alkanes, Wurtz Reaction, Wurtz-Fittig Reactions, Free radical substitutions: Halogenation relative reactivity and selectivity.

B. Carbon-Carbon pi bonds:

Formation of alkenes and alkynes by elimination reactions, Mechanism of E1, E2, E1cb reactions. Saytzeff and Hofmann eliminations.

Reactions of alkenes: Electrophilic additions their mechanisms (Markownikoff/ Anti Markownikoff addition), mechanism of oxymercuration-demercuration, hydroborationoxidation, ozonolysis, reduction (catalytic and chemical), *syn* and *anti*-hydroxylation (oxidation). 1,2-and 1,4-addition reactions in conjugated dienes, Diels-Alder reaction; Allylic and benzylic bromination and mechanism, *e.g.* propene, 1-butene, toluene, ethyl benzene.

Reactions of alkynes: Acidity, Electrophilic and Nucleophilic additions. Hydration to form carbonyl compounds, Alkylation of terminal alkynes.

C. Cycloalkanes and Conformational Analysis

Types of cycloalkanes and their relative stability, Baeyer strain theory, Conformation analysis of alkanes: Relative stability: Energy diagrams of cyclohexane and substituted cyclohexanes: Chair, Boat and Twist boat forms; Relative stability with energy diagrams. **(24 Lectures)**

Reference Books:

- Morrison, R. N. & Boyd, R. N. Organic Chemistry, Dorling Kindersley (India) Pvt.Ltd. (Pearson Education).
- Finar, I. L. Organic Chemistry (Volume 1), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- Finar, I. L. Organic Chemistry (Volume 2: Stereochemistry and the Chemistry of Natural Products), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- Eliel, E. L. & Wilen, S. H. Stereochemistry of Organic Compounds, Wiley: London, 1994.
- Kalsi, P. S. Stereochemistry Conformation and Mechanism, New Age International, 2005.
- McMurry, J.E. Fundamentals of Organic Chemistry, 7th Ed. Cengage Learning India Edition, 2013.

CHEMISTRY PRACTICAL - C3 LAB

(Credits: Practicals-02, 60 Lectures, Full Marks: 30)

1. Checking the calibration of the thermometer
2. Purification of organic compounds by crystallization using the following solvents:
   a. Water

b. Alcohol

c. Alcohol-Water

3. Determination of the melting points of above compounds and unknown organic compounds (Kjeldahl method and electrically heated melting point apparatus)

4. Effect of impurities on the melting point – mixed melting point of two unknown organic compounds

5. Determination of boiling point of liquid compounds (boiling point lower than and more than 100 °C by distillation and capillary method).

6. Chromatography

a. Separation of a mixture of two amino acids by ascending and horizontal paper chromatography

b. Separation of a mixture of two sugars by ascending paper chromatography

c. Separation of a mixture of *o*- and *p*-nitrophenol or *o*- and *p*-aminophenol by thin layer chromatography (TLC).

Reference Books

• Mann, F.G. & Saunders, B.C. *Practical Organic Chemistry*, Pearson Education (2009)
• Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. *Practical Organic Chemistry, 5th Ed.*, Pearson (2012)

CHEM02C4: PHYSICAL CHEMISTRY- II

(Credits: Theory-04, 60 Lectures, Full Marks: 70)

Chemical Thermodynamics:

Importance and scope, intensive and extensive variables; state and path functions; isolated, closed and open systems; zeroth law of thermodynamics.

First law: Concept of heat, *q*, work, *w*, internal energy, *U*, and statement of first law; enthalpy, *H*, heat changes at constant volume and constant pressure; relation between C_p and C_v using ideal gas and van der Waals equations; joule's experiment and its consequence; explanation of term $(\delta U/\delta V)_T$, calculations of *q*, *w*, ΔU and ΔH for reversible, irreversible and free expansion of gases (ideal and van der Waals) under isothermal and adiabatic conditions.

Thermochemistry: Heats of reactions: standard states; enthalpy of formation of molecules and ions and enthalpy of combustion and its applications; calculation of bond energy, bond dissociation energy and resonance energy from thermochemical data, effect of temperature (Kirchhoff's equations) and pressure on enthalpy of reactions. Adiabatic flame temperature, explosion temperature.

Second Law: Second law of thermodynamics: need for a second law, Clausius and Kelvin-Planck statements and their equivalence; Carnot's theorem, thermodynamic scale of temperature, concept of heat engine, Carnot cycle and refrigerator; Concept of entropy; Clausius inequality, entropy as a state function, second law in terms of entropy, molecular and statistical interpretation of entropy. Calculation of entropy change for reversible and irreversible processes.

Free Energy Functions: Gibbs and Helmholtz energy; variation of S, G, A with T, V, P; Free energy change and spontaneity. Relation between Joule-Thomson coefficient and other thermodynamic parameters; inversion temperature; Gibbs-Helmholtz equation; Maxwell relations; thermodynamic equation of state.

Third Law: Statement of third law, concept of residual entropy, calculation of absolute entropy of molecules, Statistical interpretation of entropy and Boltzmann equation.

(32 Lectures)

Systems of Variable Composition:

Partial molar quantities, dependence of thermodynamic parameters on composition; Gibbs- Duhem equation, Eulers theorem. Non-ideal system: Excess thermodynamic functions, idea of fugacity and activity; standard states. chemical potential of ideal mixtures, change in thermodynamic functions in mixing of ideal gases. Activity coefficient for electrolytes, Debye Huckel theory (preliminary idea).

(12 Lectures)

Chemical Equilibrium:

Criteria of thermodynamic equilibrium, degree of advancement of reaction, chemical equilibria in ideal gases, concept of fugacity. Thermodynamic derivation of relation between

Gibbs free energy of reaction and reaction quotient. Coupling of exoergic and endoergic eactions. Equilibrium constants and their quantitative dependence on temperature, pressure and concentration. Free energy of mixing and spontaneity; thermodynamic derivation of relations between the various equilibrium constants K_p, K_c and K_x. Le Chatelier principle (quantitative treatment); equilibrium between ideal gases and a pure condensed phase. **(8 Lectures)**

Solutions and Colligative Properties:

Dilute solutions; lowering of vapour pressure, Raoult's and Henry's Laws and their applications.

Thermodynamic derivation using chemical potential to derive relations between the four colligative properties [(i) relative lowering of vapour pressure, (ii) elevation of boiling point, (iii) Depression of freezing point, (iv) osmotic pressure] and amount of solute. Applications

in calculating molar masses of normal, dissociated and associated solutes in solution.

(8 Lectures)

Reference Books

- Peter, A. & Paula, J. de. Physical Chemistry 10th Ed., Oxford University Press (2014).
- Castellan, G. W. Physical Chemistry 4th Ed., Narosa (2004).
- Engel, T. & Reid, P. Physical Chemistry 3rd Ed., Prentice-Hall (2012).
- McQuarrie, D. A. & Simon, J. D. Molecular Thermodynamics Viva Books Pvt. Ltd.: New Delhi (2004).

- Assael, M. J.; Goodwin, A. R. H.; Stamatoudis, M.; Wakeham, W. A. & Will, S. Commonly Asked Questions in Thermodynamics. CRC Press: NY (2011).
- Levine, I .N. Physical Chemistry 6th Ed., Tata Mc Graw Hill (2010).
- Metz, C.R. 2000 solved problems in chemistry, Schaum Series (2006).

CHEMISTRY PRACTICAL - C4 LAB

(Credits: Practicals-02, 60 Lectures, Full Marks: 30)

Thermochemistry

(a) Determination of heat capacity of a calorimeter for different volumes using change of enthalpy data of a known system (method of back calculation of heat capacity of calorimeter from known enthalpy of solution or enthalpy of neutralization).

(b) Determination of heat capacity of the calorimeter and enthalpy of neutralization of hydrochloric acid with sodium hydroxide.

(c) Calculation of the enthalpy of ionization of ethanoic acid.

(d) Determination of heat capacity of the calorimeter and integral enthalpy (endothermic and exothermic) solution of salts.

(e) Determination of enthalpy of hydration of copper sulphate.

(f) Study of the solubility of benzoic acid in water and determination of ΔH.

Reference Books

- Khosla, B. D.; Garg, V. C. & Gulati, A., Senior Practical Physical Chemistry, R. Chand & Co.: New Delhi (2011).
- Athawale, V. D. & Mathur, P. Experimental Physical Chemistry New Age International: New Delhi (2001).

CHEM02GE2

Theory: CHEMICAL ENERGETICS, EQUILIBRIA & FUNCTIONAL ORGANIC CHEMISTRY

(Credits: Theory-04, 60 Lectures, Full Marks: 70)

Section A: Physical Chemistry

Chemical Energetics:

Review of thermodynamics and the Laws of Thermodynamics. Important principles and definitions of thermochemistry. Concept of standard state and standard enthalpies of formations, integral and differential enthalpies of solution and dilution. Calculation of bond energy, bond dissociation energy and resonance energy from thermochemical data. Variation of enthalpy of a reaction with temperature – Kirchhoff's equation. Statement of Third Law of thermodynamics and calculation of absolute entropies of substances.

(10 Lectures)

Chemical Equilibrium:

Free energy change in a chemical reaction. Thermodynamic derivation of the law of chemical equilibrium. Distinction between ΔG and ΔG^o, Le Chatelier's principle. Relationships between Kp, Kc and Kx for reactions involving ideal gases.

(8 Lectures)

Ionic Equilibria:

Strong, moderate and weak electrolytes, degree of ionization, factors affecting degree of ionization, ionization constant and ionic product of water. Ionization of weak acids and bases, pH scale, common ion effect. Salt hydrolysis-calculation of hydrolysis constant, degree of hydrolysis and pH for different salts. Buffer solutions. Solubility and solubility product of sparingly soluble salts – applications of solubility product principle.

(12 Lecture)

Section B: Organic Chemistry

Functional group approach for the following reactions (preparations & reactions) to be studied in context to their structure.

Aromatic hydrocarbons:

Preparation of benzene: from phenol, by decarboxylation, from acetylene, from benzene sulphonic acid. Reactions of benzene: Electrophilic substitution: nitration, halogenation and sulphonation. Friedel-Craft's reaction (alkylation and acylation) (upto 4 carbons on benzene). Side chain oxidation of alkyl benzenes (upto 4 carbons on benzene). **(8 Lectures)**

Alkyl and Aryl Halides

Alkyl Halides (Upto 5 Carbons) Types of Nucleophilic Substitution (S_N1, S_N2 and S_Ni) reactions.

Preparation: from alkenes and alcohols.

Reactions: hydrolysis, nitrite & nitro formation, nitrile & isonitrile formation. Williamson's ether synthesis: Elimination *vs* substitution.

Aryl Halides Preparation: (Chloro, bromo and iodo-benzene): from phenol, Sandmeyer & Gattermann reactions.

Reactions (Chlorobenzene): Aromatic nucleophilic substitution (replacement by –OH group) and effect of nitro substituent. Benzyne Mechanism: KNH_2/ liq.NH_3 (or $NaNH_2$/liq.NH_3).

Reactivity and Relative strength of C-Halogen bond in alkyl, allyl, benzyl, vinyl and aryl halides.

(8 Lectures)

Alcohols, Phenols and Ethers (Upto 5 Carbons)

Alcohols: Preparation: Preparation of 1^o, 2^o and 3^o alcohols: using Grignard reagent, Ester hydrolysis, Reduction of aldehydes, ketones, carboxylic acids and esters. Reactions: With sodium, HX (Lucas test), esterification, oxidation (with PCC, alk. $KMnO_4$, acidic dichromate, conc. HNO_3). Oppeneauer oxidation, Diols: (Upto 6 Carbons) oxidation of diols. Pinacol-Pinacolone rearrangement.

Phenols: Preparation - Cumenehydroperoxide method, from diazonium salts. Reactions: Electrophilic substitution: Nitration, halogenation and sulphonation. Reimer-Tiemann Reaction, Gattermann-Koch Reaction, Houben–Höesch Condensation, Schötten – Baümann Reaction.

Ethers (aliphatic and aromatic): Cleavage of ethers by HI.

Aldehydes and ketones (aliphatic and aromatic): (Formaldehye, acetaldehyde, acetone and benzaldehyde)

Preparation: from acid chlorides and nitriles.

Reactions – Reaction with HCN, ROH, $NaHSO_3$, NH_2-G derivatives. Iodoform test. Aldol Condensation, Cannizzaro's reaction, Wittig reaction, Benzoin condensation. Clemensen reduction and Wolff Kishner reduction. Meerwein-Pondorff-Verley reduction.

(14 Lectures)

Reference Books:

• Graham Solomon, T.W., Fryhle, C.B. & Dnyder, S.A. *Organic Chemistry,* John Wiley & Sons (2014).
• McMurry, J.E. *Fundamentals of Organic Chemistry*, 7^{th} Ed. Cengage Learning India Edition, 2013.
• Sykes, P. *A Guidebook to Mechanism in Organic Chemistry*, Orient Longman, New Delhi (1988).
• Finar, I.L. *Organic Chemistry* (Vol. I & II), E.L.B.S.
• Morrison, R.T. & Boyd, R.N. *Organic Chemistry*, Pearson, 2010.
• Bahl, A. & Bahl, B.S. *Advanced Organic Chemistry*, S. Chand, 2010.
• Barrow, G.M. *Physical Chemistry* Tata McGraw-Hill (2007).
• Castellan, G.W. *Physical Chemistry* 4th Ed. Narosa (2004).
• Kotz, J.C., Treichel, P.M. & Townsend, J.R. *General Chemistry* Cengage Learning India Pvt. Ltd., New Delhi (2009).
• Mahan, B.H. *University Chemistry* 3rd Ed. Narosa (1998).
• Petrucci, R.H. *General Chemistry* 5th Ed. Macmillan Publishing Co.: New York (1985).

GE2-Lab: (Credits: 02, 60 Lectures, Full Marks: 30)

Section A: Physical Chemistry

Thermochemistry

1. Determination of enthalpy of neutralization of hydrochloric acid with sodium hydroxide.
2. Determination of enthalpy of ionization of acetic acid.
3. Study of the solubility of benzoic acid in water and determination of ΔH.

Ionic equilibria

pH measurements Measurement of pH of different solutions like aerated drinks, fruit juices, shampoos and soaps (use dilute solutions of soaps and shampoos to prevent damage to the glass electrode) using pH-meter.

Preparation of buffer solutions:

(i) Sodium acetate-acetic acid

(ii) Ammonium chloride-ammonium hydroxide

Measurement of the pH of buffer solutions and comparison of the values with theoretical values.

Section B: Organic Chemistry

1. Purification of organic compounds by crystallization (from water and alcohol) and distillation.
2. Criteria of Purity: Determination of melting and boiling points.
3. Preparations: Mechanism of various reactions involved to be discussed. Recrystallisation, determination of melting point and calculation of quantitative yields to be done.

(a) Bromination of Phenol/Aniline

(b) Benzoylation of amines/phenols

(c) Oxime and 2,4-dinitrophenylhydrazone of aldehyde/ketone

Reference Books

• Vogel, A.I., Tatchell, A.R., Furnis, B.S., Hannaford, A.J. & Smith, P.W.G., *Textbook of Practical Organic Chemistry*, Prentice-Hall, 5th edition, 1996.
• Mann, F.G. & Saunders, B.C. *Practical Organic Chemistry* Orient-Longman, 1960.
• Khosla, B. D.; Garg, V. C. & Gulati, A. *Senior Practical Physical Chemistry*, R. Chand & Co.: New Delhi (2011).

Semester III

CHEM03C5: INORGANIC CHEMISTRY-II

(Credits: Theory-04, 60 Lectures, Full Marks: 70)

General Principles of Metallurgy

Chief modes of occurrence of metals based on standard electrode potentials. Ellingham diagrams for reduction of metal oxides using carbon and carbon monoxide as reducing agent. Electrolytic Reduction, Hydrometallurgy. Methods of purification of metals: Electrolytic Kroll process, Parting process, van Arkel-de Boer process and Mond's process, Zone refining. **(6 Lectures)**

Acids and Bases

Bronsted and Lowry's concept, solvent system concept, Lewis concept, Lux-Flood concept, relative strength of acids, hydracids and oxyacids, Pauling's rules, amphoterism, and super acids, HSAB principle, acid-base equilibria in aqueous solution, pH, buffer solutions and buffer actions, acid-base neutralization curves, acid-base indicators, choice of indicators, acid-base titrations.

Physical properties of a solvent, types of solvents and their general characteristics, reactions in non-aqueous solvents. **(12 Lectures)**

Chemistry of *s* and *p* Block Elements:

Inert pair effect, relative stability of different oxidation states, diagonal relationship and anomalous behaviour of first member of each group. Allotropy and catenation. Complex formation tendency of *s* and *p* block elements. Basic properties of halogens. Hydrides and their classification ionic, covalent and interstitial. Basic beryllium acetate and nitrate.

Study of the following compounds with emphasis on structure, bonding, preparation, properties and uses.

Boric acid and borates, boron nitrides, borohydrides (diborane) carboranes and graphitic compounds, silanes, oxides and oxoacids of nitrogen, phosphorus and chlorine. Peroxo acids of sulphur, interhalogen compounds, polyhalide ions, pseudohalogens. **(30 Lectures)**

Noble Gases:

Occurrence and uses, rationalization of inertness of noble gases, Clathrates; preparation and properties of fluorides and oxofluorides; structure and bonding of noble gas fluoro, oxo and fluoro-oxo compounds.

(6 Lectures)

Inorganic Polymers:

Types of inorganic polymers, comparison with organic polymers, synthesis, structural aspects and applications of silicones and siloxanes. Borazines, silicates and phosphazenes and polysulphates, $(SN)_n$.

(6 Lectures)

Reference Books:

- Lee, J.D. Concise Inorganic Chemistry, ELBS, 1991.
- Douglas, B.E; Mc Daniel, D.H. & Alexander, J.J. Concepts & Models of Inorganic Chemistry 3rd Ed., John Wiley Sons, N.Y. 1994.
- Greenwood, N.N. & Earnshaw. Chemistry of the Elements, Butterworth-Heinemann. 1997.
- Cotton, F.A. & Wilkinson, G. Advanced Inorganic Chemistry, Wiley, VCH, 1999.
- Rodger, G.E. Inorganic and Solid State Chemistry, Cengage Learning India Edition, 2002.
- Miessler, G. L. & Donald, A. Tarr. Inorganic Chemistry 4th Ed., Pearson, 2010. 19
- Atkin, P. Shriver & Atkins' Inorganic Chemistry 5th Ed. Oxford University Press (2010).

CHEMISTRY PRACTICAL - C5 LAB

(Credits: Practicals-02, 60 Lectures, Full Marks: 30)

(A) Iodo / Iodimetric Titrations

Principles involved in iodometric titration

(i) Estimation of Cu(II) and $K_2Cr_2O_7$ (Iodimetrically).

(ii) Estimation of available chlorine in bleaching powder iodometrically.

(B) Inorganic preparations

(i) Perchlorate salts/cuprous chloride

(ii) Preparation of Manganese (III) phosphate

(iii) Preparation of Aluminium potassium sulphate (Potash alum) orChrome alum.

Reference Book:

Mendham, J., A. I. Vogel's Quantitative Chemical Analysis 6th Ed., Pearson, 2009.

CHEM03C6: ORGANIC CHEMISTRY-II

(Credits: Theory-04, 60 Lectures, Full Marks: 70)

Chemistry of Halogenated Hydrocarbons & Reaction Kinetics:

Alkyl halides: Methods of preparation, nucleophilic substitution reactions – S_N1, S_N2 and S_Ni mechanisms, substrate structure, leaving group, nuc1eophiles including ambident nucleophiles, substitution involving NGP; relative rate & stereochemical features, nucleophilic substitution *vs*. elimination.

Aryl halides: Preparation, including preparation from diazonium salts, nucleophilic aromatic substitution; S_NAr, Benzyne mechanism.

Relative reactivity of alkyl, allyl/benzyl, vinyl and aryl halides towards nucleophilic substitution reactions.

Organometallic compounds of Mg and Li – Use in synthesis of organic compounds.

Reaction kinetics: rate const and free energy of activation, free energy profiles for one step and multistep reactions, catalyzed reactions, kinetic control and thermodynamic control, kinetic isotopic effect, principle of microscopic reversibility, Hammond postulate.

(18 Lectures)

Alcohols, Phenols, Ethers and Epoxides:

Alcohols: preparation, properties and relative reactivity of 1°, 2°, 3° alcohols, Bouveault-Blanc Reduction; Preparation and properties of glycols: Oxidation by periodic acid and lead tetraacetate, Pinacol-Pinacolone rearrangement;

Phenols: Preparation and properties; Acidity and factors effecting it, Ring substitution reactions, Reimer–Tiemann and Kolbe–Schmidt Reactions, Fries and Claisen rearrangements with mechanism;

Ethers and Epoxides: Preparation and reactions with acids. Reactions of epoxides with alcohols, ammonia derivatives and $LiAlH_4$. **(14 Lectures)**

Carbonyl Compounds:

Structure, reactivity and preparation:

Nucleophilic additions, Nucleophilic addition-elimination reactions with ammonia derivatives with mechanism; Mechanisms of Aldol and Benzoin condensation, Knoevenagel condensation, Reformatsky, Claisen-Schmidt, Perkin, Cannizzaro and Wittig reaction, Beckmann and Benzil-Benzilic acid rearrangements, haloform reaction and Baeyer Villiger oxidation, α- substitution reactions, oxidations and reductions (Clemmensen, Wolff-Kishner, $LiAlH_4$, $NaBH_4$, MPV, PDC and PGC);

Addition reactions of unsaturated carbonyl compounds: Michael addition. Active methylene compounds: Keto-enol tautomerism. Preparation and synthetic applications of diethyl malonate and ethyl acetoacetate.

(14 Lectures)

Carboxylic Acids and their Derivatives:

Preparation, physical properties and reactions of monocarboxylic acids: Typical reactions of dicarboxylic acids, hydroxy acids and unsaturated acids: succinic/phthalic, lactic, malic, tartaric, citric, maleic and fumaric acids; Preparation and reactions of acid chlorides, anhydrides, esters and amides; Comparative study of nucleophilic sustitution of acyl group -Mechanism of acidic and alkaline hydrolysis of esters, Claisen condensation, Dieckmann and Reformatsky reactions, Hofmann bromamide degradation and Curtius rearrangement.

(10 Lectures)

Sulphur containing compounds:

Preparation and reactions of thiols, thioethers and sulphonic acids. **(4 Lectures)**

Reference Books:

- Morrison, R. T. & Boyd, R. N. Organic Chemistry, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- Finar, I. L. Organic Chemistry (Volume 1), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- Graham Solomons, T.W. Organic Chemistry, John Wiley & Sons, Inc.
- McMurry, J.E. Fundamentals of Organic Chemistry, 7th Ed. Cengage Learning India Edition, 2013.

CHEMISTRY PRACTICAL - C6 LAB

(Credits: Practicals-02, 60 Lectures, Full Marks: 30)

1. Functional group tests for alcohols, phenols, carbonyl and carboxylic acid group.

2. Organic preparations:

i. Acetylation of one of the following compounds: amines (aniline, *o*-, *m*-, *p*- toluidines and *o*-, *m*-, *p*- anisidine) and phenols (β-naphthol, vanillin, salicylic acid) by any one method:

a. Using conventional method.

b. Using green approach

ii. Benzolyation of one of the following amines (aniline, *o*-, *m*-, *p*- toluidines and *o*-, *m*-, *p*-anisidine) and one of the following phenols (β-naphthol, resorcinol, pcresol) by Schötten-Baümann reaction.

iii. Oxidation of ethanol/ isopropanol (Iodoform reaction).

iv. Bromination of any one of the following:

a. Acetanilide by conventional methods

b. Acetanilide using green approach (Bromate-bromide method)

v. Nitration of any one of the following:

a. Acetanilide/nitrobenzene by conventional method

b. Salicylic acid by green approach (using ceric ammonium nitrate).

vi. Selective reduction of *meta*- dinitrobenzene to *m*-nitroaniline.

vii. Reduction of *p*-nitrobenzaldehyde by sodium borohydride.

viii. Hydrolysis of amides and esters.

ix. Semicarbazone of any one of the following compounds: acetone, ethyl methyl ketone, cyclohexanone, benzaldehyde.

x. *S*-Benzylisothiouronium salt of one each of water soluble and water insoluble acids (benzoic acid, oxalic acid, phenyl acetic acid and phthalic acid).

xi. Aldol condensation using either conventional or green method.

xii. Benzil-Benzilic acid rearrangement.

The above derivatives should be prepared using 0.5-1g of the organic compound. The solid samples must be collected and may be used for recrystallization, melting point and TLC.

Reference Books

- Mann, F.G. & Saunders, B.C. Practical Organic Chemistry, Pearson Education (2009)
- Furniss, B.S., Hannaford, A.J., Smith, P.W.G. & Tatchell, A.R. Practical Organic Chemistry, 5th Ed. Pearson (2012)
- Ahluwalia, V.K. & Aggarwal, R. Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis, University Press (2000).
- Ahluwalia, V.K. & Dhingra, S. Comprehensive Practical Organic Chemistry: Qualitative Analysis, University Press (2000).

CHEM03C7: PHYSICAL CHEMISTRY-III

(Credits: Theory-04, 60 Lectures, Full Marks: 70)

Phase Equilibria:

Concept of phases, components and degrees of freedom, derivation of Gibbs Phase Rule for nonreactive and reactive systems; Clausius-Clapeyron equation and its applications to solid liquid,

liquid-vapour and solid-vapour equilibria, phase diagram for one component systems, with applications.

Phase diagrams for systems of solid-liquid equilibria involving eutectic, congruent and incongruent melting points, solid solutions.

Three component systems, water-chloroform-acetic acid system, triangular plots.

Binary solutions: Gibbs-Duhem-Margules equation, its derivation and applications to fractional distillation of binary miscible liquids (ideal and nonideal), azeotropes, lever rule, partial miscibility of liquids, CST, miscible pairs, steam distillation.

Nernst distribution law: its derivation and applications: solvent extraction, determination of equilibrium constant.

(28 Lectures)

Chemical Kinetics

Phenomenological kinetics: degree of advancement of a reaction, reaction rate, rate constant, order and molecularity of a reaction, rate laws in terms of the advancement of a reaction, differential and integrated form of rate expressions up to second order reactions, experimental

methods of the determination of rate laws, kinetics of complex reactions (integrated rate expressions up to first order only): (i) Opposing reactions (ii) parallel reactions and (iii) consecutive reactions and their differential rate equations (steady-state approximation in reaction mechanisms) (iv) chain reactions. Differential rate law for complex reactions following reaction mechanism.

Temperature dependence of reaction rates; Arrhenius equation; activation energy. Collision theory of reaction rates, Lindemann mechanism, qualitative treatment of the theory of absolute reaction rates, primary and secondary kinetic salt effect, kinetic isotope effect.

(18 Lectures)

Catalysis:

Types of catalyst, specificity and selectivity, mechanisms of catalyzed reactions at solid surfaces; effect of particle size and efficiency of nanoparticles as catalysts. Enzyme catalysis, Michaelis-Menten mechanism, turnover number, Lineweaver-Burk plot; influence of temperature and pH acid-base catalysis. Heterogeneous catalysis (single reactant).

(6 Lectures)

Surface chemistry:

Physical adsorption, chemisorption, adsorption isotherms. nature of adsorbed state. Freundlich and Langmuir adsorption isotherm, multilayer and BET isotherm (without derivation) and applications, Gibbs adsorption isotherm and surface excess, effect of addition of substances on surface tension, surfactants and micelles and reverse micelles: applications, size and solubility. **(8 Lectures)**

Reference Books:

- Peter Atkins & Julio De Paula, Physical Chemistry 10th Ed., Oxford University Press (2014).
- Castellan, G. W. Physical Chemistry, 4th Ed., Narosa (2004).
- McQuarrie, D. A. & Simon, J. D., Molecular Thermodynamics, Viva Books Pvt. Ltd.: New Delhi (2004).
- Engel, T. & Reid, P. Physical Chemistry 3rd Ed., Prentice-Hall (2012).
- Assael, M. J.; Goodwin, A. R. H.; Stamatoudis, M.; Wakeham, W. A. & Will, S. Commonly Asked Questions in Thermodynamics. CRC Press: NY (2011).
- Zundhal, S.S. Chemistry concepts and applications Cengage India (2011).
- Ball, D. W. Physical Chemistry Cengage India (2012).
- Mortimer, R. G. Physical Chemistry 3rd Ed., Elsevier: NOIDA, UP (2009).
- Levine, I. N. Physical Chemistry 6th Ed., Tata McGraw-Hill (2011).
- Metz, C. R. Physical Chemistry 2nd Ed., Tata McGraw-Hill (2009).

CHEMISTRY PRACTICAL-C7 LAB

(Credits: Practicals-02, 60 Lectures, Full Marks: 30)

I. Determination of critical solution temperature and composition of the phenol-water system and to study the effect of impurities on it.

II. Distribution of acetic/ benzoic acid between water and cyclohexane.

III. Study the equilibrium of at least one of the following reactions by the distribution method:

(i) I_2 (aq) + I^- → I_3^- (aq) (ii) Cu^{2+} (aq) + $n NH_3$ → $Cu(NH_3)n$

IV. Study the kinetics of the following reactions.

1. Initial rate method: Iodide-persulphate reaction

2. Integrated rate method:

a. Acid hydrolysis of methyl acetate with hydrochloric acid.

b. Saponification of ethyl acetate.

V. Adsorption: Verification of the Freundlich isotherms for adsorption of acetic acid on activated charcoal.

Reference Books:

- Khosla, B. D.; Garg, V. C. & Gulati, A. Senior Practical Physical Chemistry, R. Chand & Co.: New Delhi (2011).
- Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. Experiments in Physical Chemistry 8th Ed.; McGraw-Hill: New York (2003).
- Halpern, A. M. & McBane, G. C. Experimental Physical Chemistry 3rd Ed.; W.H. Freeman & Co.: New York (2003).

CHEM03GE3.1

Theory: SOLUTIONS, PHASE EQUILIBRIA, CONDUCTANCE, ELECTROCHEMISTRY & FUNCTIONAL GROUP ORGANIC CHEMISTRY

(Credits: 04, 60 Lectures, Full Marks: 70)

Section A: Physical Chemistry

Solutions

Thermodynamics of ideal solutions: Ideal solutions and Raoult's law, deviations from Raoult's law – non-ideal solutions. Vapour pressure-composition and temperature-composition curves of ideal and non-ideal solutions. Distillation of solutions. Lever rule. Partial miscibility of liquids: Critical solution temperature; effect of impurity on partial miscibility of liquids. Nernst distribution law and its applications, solvent extraction.

(8 Lectures)

Phase Equilibria

Phases, components and degrees of freedom of a system, criteria of phase equilibrium. GibbsPhase Rule and its thermodynamic derivation. Derivation of Clausius – Clapeyron equation and its importance in phase equilibria. Phase diagrams of one-component systems (water and sulphur) and two component systems involving eutectics. **(8 Lectures)**

Conductance

Conductivity, equivalent and molar conductivity and their variation with dilution for weakand strong electrolytes. Kohlrausch law of independent migration of ions. Transference number and its experimental determination using Hittorf and Moving boundary methods. Ionic mobility. Applications of conductance measurements: determination of degree of ionization of weak electrolyte, solubility and solubility products of sparingly soluble salts, ionic product of water, hydrolysis constant of a salt. Conductometric titrations (only acid base). **(6 Lectures)**

Electrochemistry

Reversible and irreversible cells. Concept of EMF of a cell. Measurement of EMF of a cell.Nernst equation and its importance. Types of electrodes. Standard electrode potential. Electrochemical series. Thermodynamics of a reversible cell, calculation of thermodynamic properties: ΔG, ΔH and ΔS from EMF data. Calculation of equilibrium constant from EMF data. Concentration cells with transference and without transference. Liquid junction potential and salt bridge. pH determination using hydrogen electrode and quinhydrone electrode. Potentiometric titrations qualitative treatment (acid-base and oxidation-reduction only).

(8 Lectures)

Section B: Organic Chemistry

Functional group approach for the following reactions (preparations & reactions) to be studied in context to their structure.

Carboxylic acids and their derivatives

Carboxylic acids (aliphatic and aromatic)

Preparation: Acidic and Alkaline hydrolysis of esters.

Reactions: Hell – Volhard - Zelinsky Reaction.

Preparation: Acid chlorides, Anhydrides, Esters and Amides from acids and their interconversion.

Reactions: Comparative study of electrophilicity of acyl derivatives. Reformatsky Reaction, Perkin condensation. **(6 Lectures)**

Amines and Diazonium Salts

Amines (Aliphatic and Aromatic): (Upto 5 carbons)

Preparation: from alkyl halides, Gabriel Phthalimide synthesis, Hofmann Bromo amide reaction (Hofmann Degradation).

Reactions: Hofmann vs. Saytzeff elimination, Carbylamine test, Hinsberg test, with HNO_2, Schötten – Baümann Reaction. Electrophilic substitution (aniline): nitration, bromination, sulphonation.

Diazonium salts:

Preparation: from aromatic amines.

Reactions: conversion to benzene, phenol, dyes.

(6 Lectures)

Amino Acids, Peptides and Proteins:

Preparation of Amino Acids: Strecker synthesis using Gabriel phthalimide synthesis. Zwitterion, Isoelectric point and Electrophoresis.

Reactions of Amino acids: ester of –COOH group, acetylation of $–NH_2$ group, complexation, ninhydrin test.

Overview of Primary, Secondary, Tertiary and Quaternary Structure of proteins.

Determination of Primary structure of Peptides by degradation: Edmann degradation (N-terminal) and C–terminal (thiohydantoin and with carboxypeptidase enzyme). Synthesis of simple peptides (upto dipeptides) by N-protection (*t*-butyloxycarbonyl and phthaloyl) & C activating groups and Merrifield solid-phase synthesis.

(10 Lectures)

Carbohydrates:

Classification and General Properties, Glucose and Fructose (open chain and cyclic structure), Determination of configuration of monosaccharides, absolute configuration of Glucose and Fructose, Mutarotation, ascending and descending in monosaccharides. Structure of disacharrides (sucrose, cellobiose, maltose, lactose) and polysacharrides (starch and cellulose) excluding their structure elucidation. **(8 Lectures)**

Reference Books:

- Barrow, G.M. *Physical Chemistry* Tata McGraw-Hill (2007).
- Castellan, G.W. *Physical Chemistry* 4th Ed. Narosa (2004).
- Kotz, J.C., Treichel, P.M. & Townsend, J.R. *General Chemistry*, Cengage Learning India Pvt. Ltd.: New Delhi (2009).
- Mahan, B.H. *University Chemistry*, 3rd Ed. Narosa (1998).
- Petrucci, R.H. *General Chemistry*, 5th Ed., Macmillan Publishing Co.: New York (1985).
- Morrison, R. T. & Boyd, R. N. *Organic Chemistry*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- Finar, I. L. *Organic Chemistry* (*Volume 1*), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- Finar, I. L. *Organic Chemistry* (*Volume 2)*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- Nelson, D. L. & Cox, M. M. *Lehninger's Principles of Bioch*emistry *7th Ed.*, W. H. Freeman.
- Berg, J.M., Tymoczko, J.L. & Stryer, L. *Biochemistry*, W.H. Freeman, 2002.

GE3.1-Lab: (Credits: 02, 60 Lectures, Full Marks: 30)

Section A: Physical Chemistry

Distribution

Study of the equilibrium of one of the following reactions by the distribution method:

$I_2(aq) + I(aq) = I_3^-(aq)$

$Cu^{2+}(aq) + xNH_3(aq) = [Cu(NH_3)_x]^{2+}$

Phase equilibria

Determination of the critical solution temperature and composition of the phenol water system and study of the effect of impurities on it.

Conductance

1. Determination of cell constant
2. Determination of equivalent conductance, degree of dissociation and dissociation constant of a weak acid.
3. Perform the following conductometric titrations:

a. Strong acid vs. strong base

b. Weak acid vs. strong base

Potentiometry

1. Perform the following potentiometric titrations (any two):

a. Strong acid vs. strong base

b. Weak acid vs. strong base

c. Potassium dichromate vs. Mohr's salt

Section B: Organic Chemistry

I. Systematic Qualitative Organic Analysis of Organic Compounds possessing monofunctional groups (-COOH, phenolic, aldehydic, ketonic, amide, aromatic nitro, aromatic amines) and preparation of one derivative.

II.

1. Separation of amino acids by paper chromatography
2. Determination of the concentration of glycine solution by formylation method.
3. Titration curve of glycine
4. Action of salivary amylase on starch
5. Effect of temperature on the action of salivary amylase on starch.
6. Differentiation between a reducing and a nonreducing sugar.

Reference Books:

- Vogel, A.I., Tatchell, A.R., Furnis, B.S., Hannaford, A.J. & Smith, P.W.G., *Textbook of Practical Organic Chemistry*, Prentice-Hall, 5th edition, 1996.
- Mann, F.G. & Saunders, B.C. *Practical Organic Chemistry* Orient-Longman, 1960.
- Khosla, B. D.; Garg, V. C. & Gulati, A. *Senior Practical Physical Chemistry*, R. Chand & Co.: New Delhi (2011).
- Ahluwalia, V.K. & Aggarwal, R. *Comprehensive Practical Organic Chemistry*,Universities Press.

OR

CHEM03GE3.2

Theory: MOLECULES OF LIFE (Credits: 04, 60 Lectures, Full Marks: 70)

Carbohydrates

Classification of carbohydrates, reducing and non-reducing sugars, General properties of glucose and fructose, their open chain structures. Epimers, mutarotation and anomers. Determination of configuration of Glucose by Fischer's method. Cyclic structure of glucose. Haworth projections. Cyclic structure of fructose. Linkage between monosachharides, structure of disacharrides (sucrose, maltose, lactose) and polysacharrides (starch and cellulose) excluding their structure elucidation. **(10 Lectures)**

Amino Acids, Peptides and Proteins

Classification *of Amino Acids,* Zwitterion structure and Isoelectric point. Overview of Primary, Secondary, Tertiary and Quaternary structure of proteins. Determination of primary structure of peptides, determination of N-terminal amino acid (by DNFB and Edman method) and C–terminal amino acid (by thiohydantoin and with carboxypeptidase enzyme). Synthesis of simple peptides (upto dipeptides) by N-protection (*t*-butyloxycarbonyl and phthaloyl) & C-activating groups and Merrifield solid phase synthesis. **(12 Lectures)**

Enzymes and correlation with drug action

Mechanism of enzyme action, factors affecting enzyme action, Coenzymes and cofactors and their role in biological reactions, Specificity of enzyme action (including stereospecificity), Enzyme inhibitors and their importance, phenomenon of inhibition (Competitive and Noncompetitive inhibition including allosteric inhibition). Drug action-receptor theory. Structure–activity relationships of drug molecules, binding role of –OH group, -NH_2 group, double bond and aromatic ring.

(12 Lectures)

Nucleic Acids

Components of nucleic acids: Adenine, Guanine, Thymine and Cytosine (Structure only), other components of nucleic acids, Nucleosides and nucleotides (**nomenclature**), Structure of polynucleotides; Structure of DNA (Watson-Crick model) and RNA (**types of RNA**), Genetic Code, Biological roles of DNA and RNA: Replication, Transcription and Translation. **(10 Lectures)**

Lipids

Introduction to lipids, classification.

Oils and fats: Common fatty acids present in oils and fats, Omega fatty acids, Trans fats, Hydrogenation, Saponification value, Iodine number. Biological importance of triglycerides, phospholipids, glycolipids, and steroids (cholesterol). **(8 Lectures)**

Concept of Energy in Biosystems

Calorific value of food. Standard caloric content of carbohydrates, proteins and fats. Oxidation of foodstuff (organic molecules) as a source of energy for cells. Introduction to Metabolism (catabolism, anabolism), ATP: the universal currency of cellular energy, ATP hydrolysis and free energy change.

Conversion of food into energy. Outline of catabolic pathways of Carbohydrate- Glycolysis,

Fermentation, Krebs Cycle. Overview of catabolic pathways of Fats and Proteins. Interrelationships in the metabolic pathways of Proteins, Fats and Carbohydrates. **(8 Lectures)**

Reference Books:

- Morrison, R. T. & Boyd, R. N. *Organic Chemistry*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- Finar, I. L. *Organic Chemistry* (*Volume 1*), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- Finar, I. L. *Organic Chemistry* (*Volume 2)*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- Nelson, D. L. & Cox, M. M. *Lehninger's Principles of Biochemistry 7th Ed.*, W. H. Freeman.
- Berg, J.M., Tymoczko, J.L. & Stryer, L. *Biochemistry*, W.H. Freeman, 2002.

GE3.2 - LAB: (Credits: 02, 60 Lectures, Full Mars: 30)

1. Separation of amino acids by paper chromatography
2. To determine the concentration of glycine solution by formylation method.

3. Study of titration curve of glycine

4. Action of salivary amylase on starch

5. Effect of temperature on the action of salivary amylase on starch.

6. To determine the saponification value of an oil/fat.

7. To determine the iodine value of an oil/fat

8. Differentiate between a reducing/ nonreducing sugar.

9. Extraction of DNA from onion/cauliflower

10. To synthesise aspirin by acetylation of salicylic acid and compare it with the ingredient of an aspirin tablet by TLC.

Reference Books:

• Furniss, B.S.; Hannaford, A.J.; Rogers, V.; Smith, P.W.G.; Tatchell, A.R. *Vogel's Textbook of Practical Organic Chemistry*, ELBS.
• Ahluwalia, V.K. & Aggarwal, R. *Comprehensive Practical Organic Chemistry*,Universities Press.

Skill Enhancement Course (Credit: 04 each)
CHEM03SEC1.1: IT SKILLS FOR CHEMISTS

(Credits: 04, 60 Lectures, Full Marks: 100)

Mathematics

Fundamentals, mathematical functions, polynomial expressions, logarithms, the exponential function, units of a measurement, interconversion of units, constants and variables, equation of a straight line, plotting graphs.

Uncertainty in experimental techniques: Displaying uncertainties, measurements in chemistry, decimal places, significant figures, combining quantities.

Uncertainty in measurement: types of uncertainties, combining uncertainties. Statistical treatment. Mean, standard deviation, relative error. Data reduction and the propagation of errors. Graphical and numerical data reduction. Numerical curve fitting: the method of least squares (regression).

Algebraic operations on real scalar variables (e.g. manipulation of van der Waals equation in different forms).Roots of quadratic equations analytically and iteratively (e.g. pH of a weak acid). Numerical methods of finding roots (Newton-Raphson, binary –bisection, e.g. pH of a weak acid not ignoring the ionization of water, volume of a van der Waals gas, equilibrium constant expressions).

Differential calculus: The tangent line and the derivative of a function, numerical differentiation (e.g., change in pressure for small change in volume of a van der Waals gas, potentiometric titrations).

Numerical integration (Trapezoidal and Simpson's rule, e.g. entropy/enthalpy change from heat capacity data).

Computer programming:

Constants, variables, bits, bytes, binary and ASCII formats, arithmetic expressions, hierarchy of operations, inbuilt functions. Elements of the BASIC language (FORTRAN). BASIC keywords and commands. Logical and relative operators. Strings and graphics. Compiled versus interpreted languages. Debugging. Simple programs using these concepts. Matrix addition and multiplication. Statistical analysis.

BASIC programs for curve fitting, numerical differentiation and integration (Trapezoidal rule, Simpson's rule), finding roots (quadratic formula, iterative, Newton-Raphson method).

HANDS ON

Introductory writing activities: Introduction to word processor and structure drawing (ChemSketch) software. Incorporating chemical structures, chemical equations, expressions from chemistry (e.g. Maxwell-Boltzmann distribution law, Bragg's law, van der Waals equation, etc.) into word processing documents.

Handling numeric data: Spreadsheet software (Excel/Origin/Gnuplot)), creating a spreadsheet, entering and formatting information, basic functions and formulae, creating charts, tables and graphs.

Incorporating tables and graphs into word processing documents. Simple calculations, plotting graphs using a spreadsheet (Planck's distribution law, radial distribution curves for hydrogenic orbitals, gas kinetic theory- Maxwell-Boltzmann distribution curves as function of temperature and molecular weight), spectral data, pressure-volume curves of van der Waals gas (van der Waals isotherms), data from phase equilibria studies. Graphical solution of equations.

Numeric modelling: Simulation of pH metric titration curves. Excel functions LINEST and Least Squares. Numerical curve fitting (Origin), linear regression (rate constants from concentrationtime

data, molar extinction coefficients from absorbance data), numerical differentiation (e.g. handling data from potentiometric and pH metric titrations, pKa of weak acid), integration (e.g. entropy/enthalpy change from heat capacity data).

Statistical analysis: Gaussian distribution and Errors in measurements and their effect on data sets. Descriptive statistics using Excel.

Presentation: Presentation graphics (Power Point Presnttion).

Reference Books:

- McQuarrie, D. A. *Mathematics for Physical Chemistry University* Science Books (2008).
- Mortimer, R. *Mathematics for Physical Chemistry*. 3rd Ed. Elsevier (2005).
- Steiner, E. *The Chemical Maths Book* Oxford University Press (1996).
- Yates, P. *Chemical calculations.* 2nd Ed. CRC Press (2007).
- Harris, D. C. *Quantitative Chemical Analysis*. 6th Ed., Freeman (2007) Chapters 3-5.
- Levie, R. de, *How to use Excel in analytical chemistry and in general scientific data analysis*, Cambridge Univ. Press (2001) 487 pages.
- Noggle, J. H. *Physical chemistry on a Microcomputer.* Little Brown & Co. (1985).
- Venit, S.M. *Programming in BASIC: Problem solving with structure and style*. Jaico Publishing House: Delhi (1996).

OR

CHEM03SEC1.2: BASIC ANALYTICAL AND NUCLEAR CHEMISTRY

(Credits: 04, 60 Lectures, Full Marks: 100)

Introduction: Introduction to Analytical Chemistry and its interdisciplinary nature. Concept of sampling. Importance of accuracy, precision and sources of error in analytical measurements. resentation of experimental data and results, from the point of view of significant figures.

Analysis of soil: Composition of soil, Concept of pH and pH measurement, Complexometric titrations, Chelation, Chelating agents, use of indicators

a. Determination of pH of soil samples.

b. Estimation of Calcium and Magnesium ions as Calcium carbonate by complexometric titration.

Analysis of water: Definition of pure water, sources responsible for contaminating water, water sampling methods, water purification methods.

a. Determination of pH, acidity and alkalinity of a water sample.

b. Determination of dissolved oxygen (DO) of a water sample.

Chromatography: Definition, general introduction on principles of chromatography, paper chromatography, TLC etc.

a. Paper chromatographic separation of mixture of metal ion (Fe^{3+} and Al^{3+}).

b. To compare paint samples by TLC method.

Ion-exchange: Column, ion-exchange chromatography etc.

Determination of ion exchange capacity of anion / cation exchange resin (using batch procedure if use of column is not feasible).

Suggested Applications (Any one):

a. To study the use of phenolphthalein in trap cases.

b. To analyze arson accelerants.

c. To carry out analysis of gasoline.

Suggested Instrumental demonstrations:

a. Estimation of macro nutrients: Potassium, Calcium, Magnesium in soil samples by flame photometry.

b. Spectrophotometric determination of Iron in Vitamin / Dietary Tablets.

c. Spectrophotometric Identification and Determination of Caffeine and Benzoic Acid in Soft Drinks.

Radioactivity

Nuclear stability and nuclear binding energy. Nuclear forces: meson exchange theory. Nuclear models (elementary idea): Concept of nuclear quantum number, magic numbers. Nuclear Reactions: Artificial radioactivity, transmutation of elements, fission, fusion and spallation. Nuclear energy and power generation. Separation and uses of isotopes. Basic instrumentation, measurement of radioactivity, principles of isotope dilution analysis, neutron activation analysis Radio chemical methods: principles of determination of age of rocks and minerals, radio carbon dating, hazards of radiation and safety measures.

Reference Books:

- Willard, H.H., Merritt, L.L., Dean, J. & Settoe, F.A. *Instrumental Methods of Analysis*, 7th Ed. Wadsworth Publishing Company Ltd., Belmont, California, USA,1988.
- Skoog, D.A., Holler, F.J. & Crouch, S. *Principles of Instrumental Analysis*, Cengage Learning India Edition, 2007.
- Skoog, D.A.; West, D.M. & Holler, F.J. *Analytical Chemistry: An Introduction 6th Ed.*, Saunders College Publishing, Fort Worth, Philadelphia (1994).
- Harris, D. C. *Quantitative Chemical Analysis*, 9th ed. Macmillan Education, 2016.
- Dean, J. A. *Analytical Chemistry Handbook*, McGraw Hill, 2004.

- Day, R. A. & Underwood, A. L. *Quantitative Analysis*, Prentice Hall of India, 1992.
- Freifelder, D.M. *Physical Biochemistry 2nd Ed.*, W.H. Freeman & Co., N.Y. USA (1982).
- Cooper, T.G. *The Tools of Biochemistry*, John Wiley & Sons, N.Y. USA. 16 (1977).
- Vogel, A. I. *Vogel's Qualitative Inorganic Analysis 7th Ed.,* Prentice Hall, 1996.
- Mendham, J., *A. I. Vogel's Quantitative Chemical Analysis 6th Ed.,* Pearson, 2009.
- Robinson, J.W. *Undergraduate Instrumental Analysis 5th Ed.*, Marcel Dekker, Inc., New York (1995).
- Christian, G.D. *Analytical Chemistry*, 6th Ed. John Wiley & Sons, New York, 2004.
- Nuclear Chemistry by M.G. Arora, Mandip Singh.
- Essentials of Nuclear Chemistry by Hari Jeevan Arnikar.
- Textbook of Nuclear Chemistry by A. Singh, R. Singh.

Semester IV

CHEM04C8: INORGANIC CHEMISTRY-III

(Credits: Theory-04, 60 Lectures, Full Marks: 70)

Coordination Chemistry:

Werner's theory, IUPAC nomenclature of coordination compounds, isomerism in coordination compounds. Stereochemistry of complexes with 4 and 6 coordination numbers. valence bond theory (inner and outer orbital complexes), electroneutrality principle and back bonding. Crystal field theory, measurement of 10 Dq (Δo), CFSE in weak and strong fields, pairing energies, factors affecting the magnitude of 10 Dq (Δo, Δt). Octahedral vs. tetrahedral coordination, tetragonal distortions from octahedral geometry Jahn-Teller theorem, square planar geometry. Qualitative aspect of Ligand field and MO Theory.

Orbital and spin magnetic moments, spin only moments of d^n ions and their correlation with effective magnetic moments, including orbital contribution;

quenching of magnetic moment: super exchange and ferromagnetic/antiferromagnetic interactions (elementary idea with examples only); d-d transitions; L-S coupling; qualitative Orgel diagrams for $3d^1$-$3d^9$ ions and their spectroscopic ground states; selection rules for electronic spectral transitions; spectrochemical series ofligands; charge transfer spectra (elementary idea).

Chelate effect, polynuclear complexes, Labile and inert complexes. Stability constant. **(30 Lectures)**

Transition Elements:

General group trends with special reference to electronic configuration, colour, variable valency, magnetic and catalytic properties, ability to form complexes. Stability of various oxidation states and e.m.f. (Latimer diagram). Difference between the first, second and third transition series. Chemistry of Ti, V, Cr Mn, Fe and Co in various oxidation states (excluding their metallurgy). **(12 Lectures)**

Lanthanoids and Actinoids:

Electronic configuration, ionization energy, oxidation states, colour, spectral and magnetic properties, lanthanide contraction, separation of lanthanides (ion-exchange method only). **(6 Lectures)**

Bioinorganic Chemistry:

Elements of life: essential, major, trace and ultratrace elements. Basic chemical reactions in the biological systems and the role of metal ions (specially Na^+, K^+, Mg^{2+}, Ca^{2+}, $Fe^{3+/2+}$, $Cu^{2+/+}$, and Zn^{2+}). Ionophores, Sodium potassium pump. Biological functions of hemoglobin and myoglobin, cytochromes and ferredoxins, carboxypeptidase, carbonic anhydrase. Biological nitrogen fixation, Photosynthesis: Photo system-I and Photosystem-II. Toxic metal ions and their effects, chelation therapy, Pt and Au complexes as drugs (examples only), metal dependent diseases. **(12 Lectures)**

Reference Books:

- Purcell, K.F & Kotz, J.C. Inorganic Chemistry W.B. Saunders Co, 1977.
- Huheey, J.E., Inorganic Chemistry, Prentice Hall, 1993.
- Lippard, S.J. & Berg, J.M. Principles of Bioinorganic Chemistry Panima Publishing Company 1994.
- Cotton, F.A. & Wilkinson, G, Advanced Inorganic Chemistry Wiley-VCH, 1999
- Basolo, F, and Pearson, R.C. Mechanisms of Inorganic Chemistry, John Wiley & Sons, NY, 1967.
- Greenwood, N.N. & Earnshaw A. Chemistry of the Elements, Butterworth-Heinemann, 1997.

CHEMISTRY PRACTICAL –C8 LAB

(Credits: Practicals-02, 60 Lectures, Full Marks: 30)

Gravimetric Analysis:

Principles involved in gravimetric analysis (any two)

i. Estimation of nickel(II) using dimethylglyoxime (DMG).

ii. Estimation of copper as CuSCN

iii. Estimation of iron as Fe_2O_3 by precipitating iron as $Fe(OH)_3$.

iv. Estimation of Al(III) by precipitating with oxine and weighing as $Al(oxine)_3$ (aluminium oxinate).

Inorganic Preparations (any two):

i. Tetraamminecopper(II) sulphate

ii. *Cis*- and *trans*- Potassium dioxalatodiaquachromate(III)

iii. Tetraamminecarbonatocobalt(III) ion

iv. Potassium tris(oxalate)ferrate(III)

Chromatography of metal ions

Principles involved in chromatographic separations. Paper chromatographic separation of following metal ions:

i. Ni(II) and Co(II)

ii. Fe(III) and Al(III)

Reference Book:

Mendham, J., A. I. Vogel’s Quantitative Chemical Analysis 6th Ed., Pearson, 2009.

CHEM04C9: ORGANIC CHEMISTRY-III

(Credits: Theory-04, 60 Lectures, Full Marks: 30)

Nitrogen Containing Functional Groups

Preparation and important reactions of nitro and compounds, nitriles and isonitriles Amines: Effect of substituent and solvent on basicity; Preparation and properties: Gabriel phthalimide synthesis, Carbylamine reaction, Mannich reaction, Hoffmann's exhaustive methylation, Hofmann-elimination reaction; Distinction between 1°, 2° and 3° amines with Hinsberg reagent and nitrous acid.

Diazonium Salts: Preparation and their synthetic applications. **(18 Lectures)**

Polynuclear Hydrocarbons

Reactions of naphthalene phenanthrene and anthracene Structure, Preparation and structure elucidation and important derivatives of naphthalene and anthracene; Polynuclear hydrocarbons.

(8 Lectures)

Heterocyclic Compounds

Classification and nomenclature, Structure, aromaticity in 5-numbered and 6-membered rings containing one heteroatom; Synthesis, reactions and mechanism of substitution reactions of: Furan, Pyrrole (Paal-Knorr synthesis, Knorr pyrrole synthesis, Hantzsch synthesis), Thiophene, Pyridine (Hantzsch synthesis), Pyrimidine, Structure elucidation of indole, Fischer indole synthesis and Madelung synthesis), Structure elucidation of quinoline and isoquinoline, Skraup synthesis, Friedlander synthesis, Knorr quinoline synthesis, Doebner- Miller synthesis, Bischler-Napieralski reaction, Pictet-Spengler reaction, Pomeranz-Fritsch reaction.

Derivatives of furan: Furfural and furoic acid. **(22 Lectures)**

Alkaloids

Natural occurrence, General structural features, Isolation and their physiological action Hoffmann's exhaustive methylation, Emde modification, Structure elucidation and synthesis of Hygrine and Nicotine. Medicinal importance of Nicotine, Hygrine, Quinine, Morphine, Cocaine and Reserpine.

(6 Lectures)

Terpenes

Occurrence, classification, isoprene rule; Elucidation of stucture and synthesis of Citral, Neral and α-terpineol.

(6 Lectures)

Reference Books:

- Morrison, R. T. & Boyd, R. N. Organic Chemistry, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- Finar, I. L. Organic Chemistry (Volume 1), Dorling Kindersley (India) Pvt. Ltd.

(Pearson Education).
- Finar, I. L. Organic Chemistry (Volume 2: Stereochemistry and the Chemistry of Natural Products), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- Acheson, R.M. Introduction to the Chemistry of Heterocyclic compounds, John Welly & Sons (1976).
- Graham Solomons, T.W. Organic Chemistry, John Wiley & Sons, Inc.
- McMurry, J.E. Fundamentals of Organic Chemistry, 7th Ed. Cengage Learning India Edition, 2013.
- Kalsi, P. S. Textbook of Organic Chemistry 1st Ed., New Age International (P) Ltd. Pub.
- Clayden, J.; Greeves, N.; Warren, S.; Wothers, P.; Organic Chemistry, Oxford University Press.
- Singh, J.; Ali, S.M. & Singh, J. Natural Product Chemistry, Prajati Parakashan (2010).

CHEMISTRY PRACTICAL-C9 LAB

(Credits: Practicals-02, 60 Lectures, Full Marks: 30)

1. Detection of extra elements.

2. Functional group test for nitro, amine and amide groups.

3. Qualitative analysis of unknown organic compounds containing simple functional groups (alcohols, carboxylic acids, phenols and carbonyl compounds)

Reference Books

- Mann, F.G. & Saunders, B.C. Practical Organic Chemistry, Pearson Education (2009)
- Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. Practical Organic Chemistry, 5th Ed., Pearson (2012)
- Ahluwalia, V.K. & Aggarwal, R. Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis, University Press (2000).
- Ahluwalia, V.K. & Dhingra, S. Comprehensive Practical Organic Chemistry: Qualitative Analysis, University Press (2000).

CHEM04C10: PHYSICAL CHEMISTRY-IV

(Credits: Theory-04, 60 Lectures, Full Marks: 70)

General Law for charge transfer, Comparison of conduction in solutions and metals, Arrhenius theory of electrolytic dissociation. Conductivity, equivalent and molar conductivity

and their variation with dilution for weak and strong electrolytes. Molar conductivity at infinite dilution. Kohlrausch law of independent migration of ions. Structure of ionic solutions, Debye-Huckel law (with derivation), Debye-Hückel-Onsager equation, Wien effect, Debye-Falkenhagen effect, Walden's rules, Temperature and viscosity dependence of conductivity, abnormal conductivity of H^+ and OH^- ions, Grotthuss mechanism, Ionic velocities, mobilities and their determinations, transference numbers and their relation to ionic mobilities, determination of transference numbers using Hittorf and Moving Boundary methods. Applications of conductance measurement: (i) degree of dissociation of weak electrolytes, (ii) ionic product of water (iii) solubility and solubility product of sparingly soluble salts, (iv) conductometric titrations, and (v) hydrolysis constants of salts. **(20 Lectures)**

Electrochemistry

Quantitative aspects of Faraday's laws of electrolysis, rules of oxidation/reduction of ions based on half-cell potentials, applications of electrolysis in metallurgy and industry. Chemical cells, reversible and irreversible cells with examples. Electromotive force of a cell and its measurement, Nernst equation; Standard electrode (reduction) potential and its application to different kinds of half-cells. Application of EMF measurements in determining

(i) free energy, enthalpy and entropy of a cell reaction, (ii) equilibrium constants, and (iii) pH

values, using hydrogen, quinone-hydroquinone, glass and SbO/Sb_2O_3 electrodes.

Concentration cells with and without transference, liquid junction potential; determination of activity coefficients and transference numbers. Qualitative discussion of potentiometric titrations (acid-base, redox, precipitation). **(20 Lectures)**

Electrical & Magnetic Properties of Atoms and Molecules

Basic ideas of electrostatics, electric field, Gauss law, concept of electric potential, Poisson's equation, electric field due to point dipole, energy of a dipole in an electric field, polarizability (distortion and orientational), Electrostatics of dielectric media, relation between polarization and surface charge density, Clausius-Mosotti equation, estimation of orientational polarizability, Debye equation, Lorenz-Laurentz equation, Measurements of Dipole moment and molecular polarizabilities.

Spin and orbital contribution in magnetic moment, Diamagnetism, paramagnetism, ferromagnetism and anti-ferromagnetism; magnetic susceptibility and its measurement (Gouy's method, SQUID), Temperature dependence of magnetic susceptibility, Curie's equation. **(20 Lectures)**

Reference Books:

- Atkins, P.W & Paula, J.D. Physical Chemistry, 10th Ed., Oxford University Press (2014).
- Castellan, G. W. Physical Chemistry 4th Ed., Narosa (2004).
- Mortimer, R. G. Physical Chemistry 3rd Ed., Elsevier: NOIDA, UP (2009).
- Barrow, G. M., Physical Chemistry 5th Ed., Tata McGraw Hill: New Delhi (2006).
- Engel, T. & Reid, P. Physical Chemistry 3rd Ed., Prentice-Hall (2012).
- Rogers, D. W. Concise Physical Chemistry Wiley (2010).
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- Silbey, R. J.; Alberty, R. A. & Bawendi, M. G. Physical Chemistry 4th Ed., John Wiley & Sons, Inc. (2005).

CHEMISTRY PRACTICAL-C10 LAB

(Credits: Practicals-02, 60 Lectures, Full Marks: 30)

Conductometry

I. Determination of cell constant

II. Determination of equivalent conductance, degree of dissociation and dissociation constant of a weak acid.

III. Perform the following conductometric titrations:

i. Strong acid vs. strong base

ii. Weak acid vs. strong base

iii. Mixture of strong acid and weak acid vs. strong base

iv. Strong acid vs. weak base

Potentiometry

Perform the following potentiometric titrations:

i. Strong acid vs. strong base

ii. Weak acid vs. strong base

iii. Dibasic acid vs. strong base

iv. Potassium dichromate vs. Mohr's salt

Reference Books:

- Khosla, B. D.; Garg, V. C. & Gulati, A. Senior Practical Physical Chemistry, R. Chand & Co.: New Delhi (2011).
- Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. Experiments in Physical Chemistry 8th Ed.; McGraw-Hill: New York (2003).
- Halpern, A. M. & McBane, G. C. Experimental Physical Chemistry 3rd Ed.; W.H. Freeman & Co.: New York (2003).

CHEM04GE4.1

Theory: TRANSITION METAL & COORDINATION CHEMISTRY, STATES OF MATTER & CHEMICAL KINETICS

(Credits: 04, 60 Lectures, Full Marks: 70)

Section A: Inorganic Chemistry

Transition Elements (3d series)

General group trends with special reference to electronic configuration, variable valency, colour, magnetic properties and ability to form complexes and stability of various oxidation states (Latimer diagrams) for Mn, Fe and Cu.

Lanthanoids and actinoids: Electronic configurations, ionization energy, oxidation states, electronic spectra, magnetic properties, lanthanide contraction, separation of lanthanides (ion exchange method only).

(12 Lectures)

Coordination Chemistry

Valence Bond Theory (VBT): Inner and outer orbital complexes of Cr, Fe, Co, Ni and Cu (coordination numbers 4 and 6). Structural and stereoisomerism in complexes with coordination numbers 4 and 6.

Drawbacks of VBT. IUPAC system of nomenclature.

(8 Lectures)

Crystal Field Theory

Crystal field effect, octahedral symmetry. Crystal field stabilization energy (CFSE), Crystal field effects for weak and strong fields. Tetrahedral symmetry. Factors affecting the magnitude of Dq. Spectrochemical series. Comparison of CFSE for O_h and T_d complexes, Tetragonal distortion of octahedral geometry.

Jahn-Teller distortion, Square planar coordination.

(10 Lectures)

Section B: Physical Chemistry

Kinetic Theory of Gases

Postulates of Kinetic Theory of Gases and derivation of the kinetic gas equation.

Deviation of real gases from ideal behaviour, compressibility factor, causes of deviation. Van der Waals equation of state for real gases. Boyle temperature (derivation not required). Critical phenomena, critical constants and their calculation from van der Waals equation. Andrews isotherms of CO_2.

Maxwell Boltzmann distribution laws of molecular velocities and molecular energies (graphic representation – derivation not required) and their importance.

Temperature dependence of these distributions. Most probable, average and root mean square velocities (no derivation). Collision cross section, collision number, collision frequency, collision diameter and mean free path of molecules. Viscosity of gases and effect of temperature and pressure on coefficient of viscosity (qualitative treatment only). **(8 Lectures)**

Liquids

Surface tension and its determination using stalagmometer. Viscosity of a liquid and determination of coefficient of viscosity using Ostwald viscometer. Effect of temperature on surface tension and coefficient of viscosity of a liquid (qualitative treatment only).

(6 Lectures)

Solids

Forms of solids. Symmetry elements, unit cells, crystal systems, Bravais lattice types and identification of lattice planes. Laws of Crystallography - Law of constancy of interfacial angles, Law of rational indices. Miller indices. X–Ray diffraction by crystals, Bragg's law. Structures of NaCl, KCl and CsCl (qualitative treatment only). Defects in crystals. Glasses and liquid crystals.

(8 Lectures)

Chemical Kinetics

The concept of reaction rates. Effect of temperature, pressure, catalyst and other factors on reaction rates. Order and molecularity of a reaction. Derivation of integrated rate equations for zero, first and second order reactions (both for equal and unequal concentrations of reactants). Half–life of a reaction. General methods for determination of order of a reaction. Concept of activation energy and its calculation from Arrhenius equation.

Theories of Reaction Rates: Collision theory and Activated Complex theory of bimolecular reactions. Comparison of the two theories (qualitative treatment only). **(8 Lectures)**

Reference Books:

- Barrow, G.M. *Physical Chemistry* Tata McGraw-Hill (2007).
- Castellan, G.W. *Physical Chemistry* 4th Ed. Narosa (2004).
- Kotz, J.C., Treichel, P.M. & Townsend, J.R. *General Chemistry* Cengage Learning India Pvt. Ltd., New Delhi (2009).
- Mahan, B.H. *University Chemistry* 3rd Ed. Narosa (1998).
- Petrucci, R.H. *General Chemistry* 5th Ed. Macmillan Publishing Co.: New York (1985).
- Cotton, F.A. & Wilkinson, G. *Basic Inorganic Chemistry*, Wiley.
- Shriver, D.F. & Atkins, P.W. *Inorganic Chemistry*, Oxford University Press.
- Wulfsberg, G. *Inorganic Chemistry*, Viva Books Pvt. Ltd.
- Rodgers, G.E. *Inorganic & Solid State Chemistry*, Cengage Learning India Ltd., 2008.

GE4.1-Lab: (Credits: 02, 60 Lectures, Full Marks: 30)

Section A: Inorganic Chemistry

Semi-micro qualitative analysis (using H_2S or other methods) of mixtures - three ionic species (two anions and one cation or one anion and two cations, excluding insoluble salts) out of the following:

Cations : NH_4^+, Pb^{2+}, Bi^{3+}, Cu^{2+}, Cd^{2+}, Fe^{3+}, Al^{3+}, Co^{2+}, Ni^{2+}, Mn^{2+}, Zn^{2+}, Ba^{2+}, Sr^{2+}, Ca^{2+}, K^+

Anions : CO_3^{2-}, S^{2-}, SO_3^{2-}, $S_2O_3^{2-}$, NO_2^-, Cl^-, Br^-, I^-, NO_3^-, SO_4^{2-}, PO_4^{3-}, BO_3^{3-}, F^-

(Spot tests should be carried out wherever feasible)

Section B: Physical Chemistry

(I) Surface tension measurement (use of organic solvents excluded).

a) Determination of the surface tension of a liquid or a dilute solution using a stalagmometer.

b) Study of the variation of surface tension of a detergent solution with concentration.

(II) Viscosity measurement (use of organic solvents excluded).

a) Determination of the relative and absolute viscosity of a liquid or dilute solution using an Ostwald's viscometer.

b) Study of the variation of viscosity of an aqueous solution with concentration of solute.

(III) Chemical Kinetics

Study the kinetics of the following reactions.

Integrated rate method:

a. Acid hydrolysis of methyl acetate with hydrochloric acid.

b. Saponification of ethyl acetate.

c. Compare the strengths of HCl and H_2SO_4 by studying kinetics of hydrolysis of ester.

Reference Books:

• Svehla, G. *Vogel's Qualitative Inorganic Analysis*, Pearson Education, 2012.
• Mendham, J. *Vogel's Quantitative Chemical Analysis*, Pearson, 2009.
• Khosla, B. D.; Garg, V. C. & Gulati, A. *Senior Practical Physical Chemistry*, R. Chand & Co.: New Delhi (2011).

OR

CHEM04GE4.2

Theory: QUANTUM CHEMISTRY, SPECTROSCOPY & PHOTOCHEMISTRY

(Credits: 04, 60 Lectures, Full Marks: 70)

Quantum Chemistry

Postulates of quantum mechanics, quantum mechanical operators, Schrödinger equation and its application to free particle and "particle-in-a-box" (rigorous treatment), quantization of energy levels, zero-point energy and Heisenberg Uncertainty principle; wavefunctions, probability distribution functions, nodal properties, Extension to two and three dimensional boxes, separation of variables, degeneracy. Qualitative treatment of simple harmonic oscillator model of vibrational motion: Setting up of Schrödinger equation and discussion of solution and wavefunctions. Vibrational energy of diatomic molecules and zero-point energy.

Angular momentum: Commutation rules, quantization of square of total angular momentum and z-component.

Rigid rotator model of rotation of diatomic molecule. Schrödinger equation, transformation to spherical polar coordinates. Separation of variables. Spherical harmonics. Discussion of solution.

Qualitative treatment of hydrogen atom and hydrogen-like ions: setting up of Schrödinger equation in spherical polar coordinates, radial part, quantization of energy (only final energy expression). Average and most probable distances of electron from nucleus.

Setting up of Schrödinger equation for many-electron atoms (He, Li). Need for approximation methods. Statement of variation theorem and application to simple systems (particle-in-a-box, harmonic oscillator, hydrogen atom). **(24 Lectures)**

Molecular Spectroscopy:

Interaction of electromagnetic radiation with molecules and various types of spectra.

Rotation spectroscopy: Selection rules, intensities of spectral lines, determination of bond lengths of diatomic and isotopic substitution.

Vibrational spectroscopy: Classical equation of vibration, computation of force constant, amplitude of diatomic molecular vibrations, anharmonicity, Morse potential, dissociation energies, fundamental frequencies, overtones, hot bands, degrees of freedom for polyatomic molecules, modes of vibration, concept of group frequencies.

Raman spectroscopy: Qualitative treatment of Rotational Raman effect; Vibrational Raman spectra, Stokes and anti-Stokes lines; their intensity difference, rule of mutual exclusion.

Electronic spectroscopy: Franck-Condon principle, electronic transitions, singlet and triplet states, fluorescence and phosphorescence.

Nuclear Magnetic Resonance (NMR) spectroscopy: Principles of NMR spectroscopy, Larmor precession, chemical shift and interpretation of PMR spectra of organic molecules.

Electron Spin Resonance (ESR) spectroscopy: Its principle, ESR of simple radicals. **(24 Lectures)**

Photochemistry

Characteristics of electromagnetic radiation, Lambert-Beer's law and its limitations, physical significance of absorption coefficients. Laws of photochemistry, quantum yield, actinometry, examples of low and high quantum yields, photochemical equilibrium and the differential rate of photochemical reactions, photosensitised reactions. Role of photochemical reactions in biochemical processes, photostationary states, chemiluminescence. **(12 Lectures)**

Reference Books:

• Banwell, C. N. & McCash, E. M. *Fundamentals of Molecular Spectroscopy* 4th Ed. Tata McGraw-Hill: New Delhi (2006).
• Chandra, A. K. *Introductory Quantum Chemistry* Tata McGraw-Hill (2001).
• House, J. E. *Fundamentals of Quantum Chemistry* 2nd Ed. Elsevier: USA (2004).
• Lowe, J. P. & Peterson, K. *Quantum Chemistry*, Academic Press (2005).
• Kakkar, R. *Atomic & Molecular Spectroscopy*: *Concepts & Applications*, Cambridge University Press (2015).

GE4.2 LAB: (Credits: 02, 60 Lectures, Full Marks: 30)

UV/Visible spectroscopy

1. Study the 200-500 nm absorbance spectra of $KMnO_4$ and $K_2Cr_2O_7$ (in 0.1 M H_2SO_4) and determine the λ_{max} values. Calculate the energies of the two transitions in different units (J molecule^{-1}, kJ mol^{-1}, cm^{-1}, eV).

2. Study the pH-dependence of the UV-Vis spectrum (200-500 nm) of $K_2Cr_2O_7$.

3. Record the 200-350 nm UV spectra of the given compounds (acetone, acetaldehyde, 2-propanol, acetic acid) in water.

Colorimetry

1. Verify Lambert-Beer's law and determine the concentration of $CuSO_4$/$KMnO_4$/$K_2Cr_2O_7$ in a solution of unknown concentration.

2. Determine the concentrations of $KMnO_4$and $K_2Cr_2O_7$ in a mixture.

3. Determine the dissociation constant of an indicator (phenolphthalein).

Reference Books

• Mendham, J. *Vogel's Quantitative Chemical Analysis*, Pearson, 2009.
• Khosla, B. D.; Garg, V. C. & Gulati, A., *Senior Practical Physical Chemistry*, R. Chand & Co.: New Delhi (2011).
• Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. *Experiments in Physical Chemistry 8th Ed.;* McGraw-Hill: New York (2003).
• Halpern, A. M. & McBane, G. C. *Experimental Physical Chemistry 3rd Ed.;* W.H. Freeman & Co.: New York (2003).

Skill Enhancement Course (Credit: 04 each)
CHEM04SEC2.1: GREEN METHODS IN CHEMISTRY

(Credits: 04, 60 Lectures, Full Marks: 100)

Theory:

Theory and Hand-on Experiments

Introduction: Definitions of Green Chemistry. Brief introduction of twelve principles of Green Chemistry, with examples, special emphasis on atom economy, reducing toxicity, green solvents, Green Chemistry and catalysis and alternative sources of energy, Green energy and sustainability

The following Real world Cases in Green Chemistry should be discussed:

Surfactants for carbon dioxide – Replacing smog producing and ozone depleting solvents with CO_2 for precision cleaning and dry cleaning of garments.

Designing of environmentally safe marine antifoulant.

Rightfit pigment: Synthetic azo pigments to replace toxic organic and inorganic pigments.

An efficient, green synthesis of a compostable and widely applicable plastic (poly lactic acid) made from corn.

Practicals

Preparation and characterization of biodiesel from vegetable oil.

Extraction of D-limonene from orange peel using liquid CO_2 prepared from dry ice.

Mechano chemical solvent free synthesis of azomethine.

Solvent free, microwave assisted one pot synthesis of phthalocyanine complex of copper (II).

Reference Books:

- Anastas, P.T. & Warner, J.K. *Green Chemistry- Theory and Practical*, Oxford University Press (1998).
- Matlack, A.S. *Introduction to Green Chemistry*, Marcel Dekker (2001).
- Cann, M.C. & Connely, M.E. *Real-World cases in Green Chemistry*, American Chemical Society, Washington (2000).
- Ryan, M.A. & Tinnesand, M. *Introduction to Green Chemistry*, American Chemical Society, Washington (2002).
- Sharma, R.K.; Sidhwani, I.T. & Chaudhari, M.K. *Green Chemistry Experiments: A monograph* I.K. International Publishing House Pvt Ltd. New Delhi, Bangalore.
- Lancaster, M. *Green Chemistry: An introductory text* RSC publishing, 2nd Edition.
- Sidhwani, I.T., Saini, G., Chowdhury, S., Garg, D., Malovika, Garg, N. Wealth from waste: A green method to produce biodiesel from waste cooking oil and generation of useful products from waste further generated *"A Social Awareness Project", Delhi University Journal of Undergraduate Research and Innovation*, **1(1)**: 2015.

OR

CHEM04SEC2.2: PHARMACEUTICAL CHEMISTRY

(Credits: 04, 60 Lectures, Full Marks: 100)

Theory:

Drugs & Pharmaceuticals

Drug discovery, design and development; Basic Retrosynthetic approach. Synthesis of the representative drugs of the following classes: analgesics agents, antipyretic agents, anti-inflammatory agents (Aspirin, paracetamol, lbuprofen); antibiotics (Chloramphenicol); antibacterial and antifungal agents (Sulphonamides; Sulphanethoxazol, Sulphacetamide, Trimethoprim); antiviral agents (Acyclovir), Central Nervous System agents (Phenobarbital, Diazepam),Cardiovascular (Glyceryl trinitrate), antilaprosy (Dapsone), HIV-AIDS related drugs (AZT- Zidovudine).

Fermentation

Aerobic and anaerobic fermentation. Production of (i) Ethyl alcohol and citric acid, (ii) Antibiotics; Penicillin, Cephalosporin, Chloromycetin and Streptomycin, (iii) Lysine, Glutamic acid, Vitamin B2, Vitamin B12 and Vitamin C.

Practicals

1. Preparation of Aspirin and its analysis.
2. Preparation of magnesium bisilicate (Antacid).

Reference Books:

• Patrick, G. L. *Introduction to Medicinal Chemistry*, *Oxford University* Press, UK, 2013.
• Singh, H. & Kapoor, V.K. *Medicinal and Pharmaceutical Chemistry*, Vallabh Prakashan, Pitampura, New Delhi, 2012.
• Foye, W.O., Lemke, T.L. & William, D.A.: *Principles of Medicinal Chemistry*, 4th ed., B.I. Waverly Pvt. Ltd. New Delhi.

Semester V

CHEM05C11: ORGANIC CHEMISTRY-IV

(Credits: Theory-04, 60 Lectures, Full Marks: 70)

Nucleic Acids

Components of nucleic acids, Nucleosides and nucleotides;

Structure, synthesis and reactions of: Adenine, Guanine, Cytosine, Uracil and Thymine; Structure of polynucleotides. **(9 Lectures)**

Amino Acids, Peptides and Proteins

Amino acids, Peptides and their classification.

α-Amino Acids - Synthesis, ionic properties and reactions. Zwitterions, pKa values, isoelectric point and electrophoresis;

Study of peptides: determination of their primary structures-end group analysis, methods of peptide synthesis. Synthesis of peptides using N-protecting, C-protecting and C-activating groups -Solid-phase synthesis.

(16 Lectures)

Enzymes

Introduction, classification and characteristics of enzymes. Salient features of active site of enzymes.

Mechanism of enzyme action (taking trypsin as example), factors affecting enzyme action, coenzymes and cofactors and their role in biological reactions, specificity of enzyme action (including stereospecificity), enzyme inhibitors and their importance, phenomenon of inhibition (competitive, uncompetitive and non-competitive inhibition including allosteric inhibition). **(8 Lectures)**

Lipids

Introduction to oils and fats; common fatty acids present in oils and fats, Hydrogenation of fats and oils, Saponification value, acid value, iodine number. Reversion and rancidity. **(8 Lectures)**

Concept of Energy in Biosystems

Cells obtain energy by the oxidation of foodstuff (organic molecules).

Introduction to metabolism (catabolism, anabolism).

ATP: The universal currency of cellular energy, ATP hydrolysis and free energy change. Agents for transfer of electrons in biological redox systems: NAD+, FAD. Conversion of food to energy: Outline of catabolic pathways of carbohydrate-glycolysis, fermentation, Kreb's cycle.

Overview of catabolic pathways of fat and protein.

Interrelationship in the metabolic pathways of protein, fat and carbohydrate. Caloric value of food, standard caloric content of food types. **(7 Lectures)**

Pharmaceutical Compounds: Structure and Importance

Classification, structure and therapeutic uses of antipyretics: Paracetamol (with synthesis), Analgesics: Ibuprofen (with synthesis), Antimalarials: Chloroquine (with synthesis). An elementary treatment of Antibiotics and detailed study of chloramphenicol, Medicinal values of curcumin (haldi), azadirachtin (neem), vitamin C and antacid (ranitidine). **(12 Lectures)**

Reference Books:

- Berg, J.M., Tymoczko, J.L. & Stryer, L. (2006) Biochemistry. 6th Ed. W.H. Freeman and Co.
- Nelson, D.L., Cox, M.M. & Lehninger, A.L. (2009) Principles of Biochemistry. IV Edition. W.H. Freeman and Co.
- Murray, R.K., Granner, D.K., Mayes, P.A. & Rodwell, V.W. (2009) Harper's Illustrated Biochemistry. XXVIII edition. Lange Medical Books/ McGraw-Hill.

CHEMISTRY PRACTICAL-C11 LAB

(Credits: Practicals-02, 60 Lectures, Full Marks: 30)

1. Estimation of glycine by Sorenson's formalin method.
2. Study of the titration curve of glycine.
3. Estimation of proteins by Lowry's method.
4. Study of the action of salivary amylase on starch at optimum conditions.
5. Effect of temperature on the action of salivary amylase.
6. Saponification value of an oil or a fat.
7. Determination of Iodine number of an oil/ fat.
8. Isolation and characterization of DNA from onion/ cauliflower/peas.

Reference Books:

- Manual of Biochemistry Workshop, 2012, Department of Chemistry, University of Delhi.
- Arthur, I. V. Quantitative Organic Analysis, Pears

CHEM05C12: PHYSICAL CHEMISTRY V

(Credits: Theory-04, 60 Lectures, Full Marks: 70)

Quantum Chemistry

Breakdown of classical ideas – Line Spectra, black body (or cavity) radiation, Planck's quantization, photoelectric effect, Elementary idea of Bohr Theory, Compton scattering for relativistic (preliminary idea only); wave properties of particles: de Broglie hypothesis and the concept of matter waves, Davisson-Germer experiment, nature of matter waves: group and phase velocities and the idea of a wave packet; Heisenberg uncertainty principle and its relation to the measurement process, Differentiation of small and large particles on the basis of Uncertainty Principle, necessity of more general theory.

Time-independent form of the Schrödinger equation; probabilistic interpretation of the wave function; conditions for acceptability of wave functions.

Postulates of quantum mechanics, quantum mechanical operators, Schrödinger equation and its application to free particle and "particle-in-a-box" (rigorous treatment), quantization of nergy levels, zero-point energy and Heisenberg Uncertainty principle; wavefunctions, probability distribution functions, nodal properties, Extension to two and three dimensional boxes, separation of variables, degeneracy.

Qualitative treatment of simple harmonic oscillator model of vibrational motion: Setting up of Schrödinger equation and discussion of solution and wavefunctions. Vibrational energy of diatomic molecules and zero-point energy.

Angular momentum: Commutation rules, quantization of square of total angular momentum and z-component.

Rigid rotator model of rotation of diatomic molecule. Schrödinger equation, transformation to spherical polar coordinates. Separation of variables. Spherical harmonics. Discussion of solution.

Qualitative treatment of hydrogen atom and hydrogen-like ions: setting up of Schrödinger equation in spherical polar coordinates, radial part, quantization of energy (only final energy expression). Average and most probable distances of electron from nucleus.

Setting up of Schrödinger equation for many-electron atoms (He, Li). Need for approximation methods. Statement of variation theorem and application to simple systems (particle-in-a-box, harmonic oscillator, hydrogen atom).

Chemical bonding: Covalent bonding, valence bond and molecular orbital approaches, LCAO-MO treatment of H_2^+.

Bonding and antibonding orbitals. Qualitative extension to H_2. Comparison of LCAO-MO and VB treatments of H_2 (only wavefunctions, detailed solution not required) and their limitations. Refinements of the two approaches (Configuration Interaction for MO, ionic terms in VB). Qualitative description of LCAO-MO treatment of homonuclear diatomic molecules.

(28 Lectures)

Molecular Spectroscopy:

Interaction of electromagnetic radiation with molecules and various types of spectra; Born-Oppenheimer approximation (qualitative idea).

Rotation spectroscopy: Selection rules, intensities of spectral lines, determination of bond lengths of diatomic and linear triatomic molecules, isotopic substitution.

Vibrational spectroscopy: Classical equation of vibration, computation of force constant, amplitude of diatomic molecular vibrations, anharmonicity, Morse potential, dissociation energies, fundamental frequencies, overtones, hot bands, degrees of freedom for polyatomic molecules, modes of vibration, concept of group frequencies. Vibration-rotation spectroscopy: diatomic vibrating rotator, P, Q, R branches.

Raman spectroscopy: Qualitative treatment of Rotational Raman effect; Effect of nuclear spin, Vibrational Raman spectra, Stokes and anti-Stokes lines; their intensity difference, rule of mutual exclusion.

Electronic spectroscopy: Franck-Condon principle, electronic transitions, singlet and triplet states, fluorescence and phosphorescence, dissociation and predissociation, calculation of electronic transitions of polyenes using free electron model.

Nuclear Magnetic Resonance (NMR) spectroscopy: Principles of NMR spectroscopy, Larmor precession, chemical shift and low resolution spectra, different scales, spin-spin coupling and high resolution spectra, interpretation of PMR spectra of organic molecules. Electron Spin Resonance (ESR) spectroscopy: Its principle, hyperfine structure, ESR of simple radicals.

(24 Lectures)

Photochemistry

Characteristics of electromagnetic radiation, Lambert-Beer's law and its limitations, physical significance of absorption coefficients. Laws, of photochemistry, quantum yield, actinometry, examples of low and high quantum yields, photochemical equilibrium and the differential rate of photochemical reactions, photosensitised reactions, quenching, chemiluminescence. Role of photochemical reactions in biochemical processes. Photochemical Reactions: kinetics of HI decomposition, H_2-Br_2 reaction, dimerization of anthracene, photostationary state.

(8 Lectures)

Reference Books:

- Banwell, C. N. & McCash, E. M. Fundamentals of Molecular Spectroscopy 4th Ed. Tata McGraw-Hill: New Delhi (2006).
- Chandra, A. K. Introductory Quantum Chemistry Tata McGraw-Hill (2001).
- House, J. E. Fundamentals of Quantum Chemistry 2nd Ed. Elsevier: USA (2004).
- Kakkar, R. Atomic & Molecular Spectroscopy: Concepts & Applications, Cambridge University Press (2015).
- Lowe, J. P. & Peterson, K. Quantum Chemistry, Academic Press (2005).

CHEMISTRY PRACTICAL-C 12 LAB

(Credits: Practicals-02, 60 Lectures, Full Marks: 30)

UV/Visible spectroscopy

I. Study the 200-500 nm absorbance spectra of KMnO4 and $K_2Cr_2O_7$ (in 0.1 M H_2SO_4) and determine the λmax values. Calculate the energies of the two transitions in different units (J molecule^{-1}, kJ mol^{-1}, cm^{-1}, eV).

II. Study the pH-dependence of the UV-Vis spectrum (200-500 nm) of $K_2Cr_2O_7$.

III. Record the 200-350 nm UV spectra of the given compounds (acetone, acetaldehyde, 2-propanol, acetic acid) in water. Comment on the effect of structure on the UV spectra of organic compounds.

Colourimetry

I. Verify Lambert-Beer's law and determine the concentration of $CuSO_4$/$KMnO_4$/$K_2Cr_2O_7$ in a solution of unknown concentration

II. Study the kinetics of iodination of propanone in acidic medium.

III. Determine the amount of iron present in a sample using 1,10-phenathroline.

IV. Determine the dissociation constant of an indicator (phenolphthalein).

V. Study the kinetics of interaction of crystal violet/ phenolphthalein with sodium hydroxide.

DMG, glycine) by substitution method.

Reference Books

- Khosla, B. D.; Garg, V. C. & Gulati, A., Senior Practical Physical Chemistry, R. Chand & Co.: New Delhi (2011).
- Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. Experiments in Physical Chemistry 8th Ed.; McGraw-Hill: New York (2003).
- Halpern, A. M. & McBane, G. C. Experimental Physical Chemistry 3rd Ed.; W.H. Freeman & Co.: New York (2003).

CHEMISTRY-DSE 1 and 2 (ELECTIVES)

Credit: 4 + 2

CHEM05DSE:

1. APPLICATIONS OF COMPUTERS IN CHEMISTRY

(Credits: Theory-04, 60 Lectures, Full Marks: 70)

Basics:

Constants, variables, bits, bytes, binary and ASCII formats, arithmetic expressions, hierarchy of operations, inbuilt functions. Elements of the BASIC language. BASIC keywords and commands. Logical and relative operators. Strings and graphics. Compiled versus interpreted languages. Debugging. Simple programs using these concepts. Matrix addition and multiplication. Statistical analysis.

Numerical methods:

Roots of equations: Numerical methods for roots of equations: Quadratic formula, iterative method, Newton-Raphson method, Binary bisection and Regula-Falsi.

Differential calculus: Numerical differentiation.

Integral calculus: Numerical integration (Trapezoidal and Simpson's rule), probability distributions and mean values.

Simultaneous equations: Matrix manipulation: addition, multiplication. Gauss-Siedal method.

Interpolation, extrapolation and curve fitting: Handling of experimental data.

Conceptual background of molecular modelling: Potential energy surfaces. Elementary ideas of molecular mechanics and practical MO methods.

Reference Books:

- Harris, D. C. *Quantitative Chemical Analysis*. 6th Ed., Freeman (2007) Chapters 3-5.
- Levie, R. de, *How to use Excel in analytical chemistry and in general scientific data analysis*, Cambridge Univ. Press (2001) 487 pages.
- Noggle, J. H. *Physical chemistry on a Microcomputer.* Little Brown & Co. (1985).
- Venit, S.M. *Programming in BASIC: Problem solving with structure and style.* Jaico Publishing House: Delhi (1996).

DSE LAB: APPLICATIONS OF COMPUTERS IN CHEMISTRY

(Credits: Practicals-02 60 Lectures, Full Marks: 30)

Computer programs based on numerical methods for

1. Roots of equations: (e.g. volume of van der Waals gas and comparison with ideal gas, pH of a weak acid).

2. Numerical differentiation (e.g., change in pressure for small change in volume of a van der Waals gas, potentiometric titrations).

3. Numerical integration (e.g. entropy/ enthalpy change from heat capacity data), probability distributions (gas kinetic theory) and mean values.

4. Matrix operations. Application of Gauss-Siedel method in colourimetry.

5. Simple exercises using molecular visualization software.

Reference Books:

- McQuarrie, D. A. *Mathematics for Physical Chemistry* University Science Books (2008).
- Mortimer, R. *Mathematics for Physical Chemistry*. 3rd Ed. Elsevier (2005).
- Steiner, E. *The Chemical Maths Book* Oxford University Press (1996).
- Yates, P. *Chemical Calculations*. 2nd Ed. CRC Press (2007).
- Harris, D. C. *Quantitative Chemical Analysis*. 6th Ed., Freeman (2007) Chapters 3-5.
- Levie, R. de, *How to use Excel in analytical chemistry and in general scientific data analysis*,Cambridge Univ. Press (2001) 487 pages.
- Noggle, J. H. *Physical Chemistry on a Microcomputer.* Little Brown & Co. (1985).
- Venit, S.M. *Programming in BASIC: Problem solving with structure and style.* Jaico Publishing House: Delhi (1996).

2. CHEMISTRY-DSE: POLYMER CHEMISTRY

(Credits: Theory-06, 60 Lectures, Full Marks: 70)

Introduction and history of polymeric materials:

Different schemes of classification of polymers, Polymer nomenclature, Molecular forces and chemical bonding in polymers, Texture of Polymers. **(4 Lectures)**

Functionality and its importance:

Criteria for synthetic polymer formation, classification of polymerization processes, Relationships between functionality, extent of reaction and degree of polymerization. Bifunctional systems, Poly-functional systems.

(8 Lectures)

Kinetics of Polymerization:

Mechanism and kinetics of step growth, radical chain growth, ionic chain (both cationic and anionic) and coordination polymerizations, Mechanism and kinetics of copolymerization, polymerization techniques.

(8 lectures)

Crystallization and crystallinity:

Determination of crystalline melting point and degree of crystallinity, Morphology of crystalline polymers, Factors affecting crystalline melting point. **(4 Lectures)**

Nature and structure of polymers-Structure Property relationships. **(2 Lectures)**

Determination of molecular weight of polymers (*Mn*, *Mw*, etc) by end group analysis, viscometry, light scattering and osmotic pressure methods. Molecular weight distribution and its significance. Polydispersity index. **(8 Lectures)**

Glass transition temperature (Tg) and determination of Tg, Free volume theory, WLF equation, Factors affecting glass transition temperature (Tg). **(8 Lectures)**

Polymer Solution – Criteria for polymer solubility, Solubility parameter, Thermodynamics of polymer solutions, entropy, enthalpy, and free energy change of mixing of polymers solutions, Flory- Huggins theory, Lower and Upper critical solution temperatures. **(8 Lectures)**

Properties of Polymers (Physical, thermal, Flow & Mechanical Properties). Brief introduction to preparation, structure, properties and application of the following polymers: polyolefins, polystyrene and styrene copolymers, poly(vinyl chloride) and related polymers, poly(vinyl acetate) and related polymers, acrylic polymers, fluoro polymers, polyamides and related polymers. Phenol formaldehyde resins (Bakelite, Novalac), polyurethanes, silicone polymers, polydienes, Polycarbonates, Conducting Polymers, [polyacetylene, polyaniline, poly(p-phenylene sulphide polypyrrole, polythiophene)].

(10 Lectures)

Reference Books:

- R.B. Seymour & C.E. Carraher: *Polymer Chemistry: An Introduction*, Marcel Dekker, Inc. New York, 1981.
- G. Odian: *Principles of Polymerization*, 4th Ed. Wiley, 2004.
- F.W. Billmeyer: *Textbook of Polymer Science*, 2nd Ed. Wiley Interscience, 1971.
- P. Ghosh: Polymer Science & Technology, Tata McGraw-Hill Education, 1991.
- R.W. Lenz: *Organic Chemistry of Synthetic High Polymers.* Interscience Publishers, New York, 1967.

DSE LAB: POLYMER CHEMISTRY

(Credits: Practicals-02, 60 Lectures, Full Marks: 30)

1. **Polymer synthesis**

1. Free radical solution polymerization of styrene (St) / Methyl Methacrylate (MMA) / Methyl Acrylate (MA) / Acrylic acid (AA).

a. Purification of monomer

b. Polymerization using benzoyl peroxide (BPO) / 2,2’-azo-bis-isobutylonitrile (AIBN)

2. Preparation of nylon 66/6

1. Interfacial polymerization, preparation of polyester from isophthaloyl chloride (IPC) and phenolphthalein

a. Preparation of IPC

b. Purification of IPC

c. Interfacial polymerization

3. Redox polymerization of acrylamide

4. Precipitation polymerization of acrylonitrile

5. Preparation of urea-formaldehyde resin

6. Preparations of novalac resin/ resold resin.

7. Microscale Emulsion Polymerization of Poly(methylacrylate).

Polymer characterization

1. Determination of molecular weight by viscometry:

(a) Polyacrylamide-aq.NaNO2 solution

(b) (Poly vinyl proplylidine (PVP) in water

2. Determination of the viscosity-average molecular weight of poly(vinyl alcohol) (PVOH) and the fraction of "head-to-head" monomer linkages in the polymer.

3. Determination of molecular weight by end group analysis: Polyethylene glycol (PEG) (OH group).

4. Testing of mechanical properties of polymers.

5. Determination of hydroxyl number of a polymer using colorimetric method.

Polymer analysis

1. Estimation of the amount of HCHO in the given solution by sodium sulphite method

2. Instrumental Techniques

3. IR studies of polymers

4. DSC analysis of polymers

5. Preparation of polyacrylamide and its electrophoresis

*at least 7 experiments to be carried out.

Reference Books:

- M.P. Stevens, *Polymer Chemistry: An Introduction*, 3rd Ed., Oxford University Press, 1999.
- H.R. Allcock, F.W. Lampe & J.E. Mark, *Contemporary Polymer Chemistry*, 3rd ed. Prentice-Hall (2003)
- F.W. Billmeyer, *Textbook of Polymer Science*, 3rd ed. Wiley-Interscience (1984)
- J.R. Fried, *Polymer Science and Technology*, 2nd ed. Prentice-Hall (2003)
- P. Munk & T.M. Aminabhavi, *Introduction to Macromolecular Science*, 2nd ed. John Wiley & Sons (2002)
- L. H. Sperling, *Introduction to Physical Polymer Science*, 4th ed. John Wiley & Sons (2005)
- M.P. Stevens, *Polymer Chemistry: An Introduction* 3rd ed. Oxford University Press (2005).
- Seymour/ Carraher's Polymer Chemistry, 9th ed. by Charles E. Carraher, Jr. (2013).

3. CHEMISTRY-DSE: ANALYTICAL METHODS IN CHEMISTRY

(Credits: Theory-04, 60 Lectures, Full Marks: 70)

Qualitative and quantitative aspects of analysis:

Sampling, evaluation of analytical data, errors, accuracy and precision, methods of their expression, normal law of distribution of errors, statistical test of data; F, Q and t test, rejection of data and confidence intervals.

(6 Lectures)

Optical methods of analysis:

Origin of spectra, interaction of radiation with matter, fundamental laws of spectroscopy and selection rules, Beer-Lambert's law and its validity.

UV-Visible Spectrometry: Basic principles of instrumentation (choice of source, monochromator and detector) for single and double beam instrument;

Basic principles of quantitative analysis: estimation of metal ions from aqueous solution, geometrical isomers, keto-enol tautomers. Determination of composition of metal complexes

using Job's method of continuous variation and mole ratio method.

Infrared Spectrometry: Basic principles of instrumentation (choice of source, monochromator & detector) for single and double beam instrument; sampling techniques. Structural illustration through interpretation of data, Effect and importance of isotope substitution.

Flame Atomic Absorption and Emission Spectrometry: Basic principles of instrumentation (choice of source, monochromator, detector, choice of flame and Burner designs. Techniques of atomization and sample introduction; Method of background correction, sources of chemical interferences and their method of removal. Techniques for the quantitative estimation of trace level of metal ions from water samples.

(24 Lectures)

Thermal methods of analysis:

Theory of thermogravimetry (TG), DTA & DSC principles, basic principle of TG instrumentation. Techniques for quantitative estimation of Ca and Mg from their mixture. **(4 Lectures)**

Electroanalytical methods:

Classification of electroanalytical methods, basic principle of pH metric, potentiometric and conductometric titrations. Techniques used for the determination of equivalence points. Techniques used for the determination of pKa values. Linear scan voltametry (LSV), Polarography and Cyclic voltametry, Coulometry, Electrogravimetry. **(10 Lectures)**

Separation techniques:

Solvent extraction: Classification, principle and efficiency of the technique. Mechanism of extraction: extraction by solvation and chelation.

Technique of extraction: batch, continuous and counter current extractions.

Qualitative and quantitative aspects of solvent extraction: extraction of metal ions from aqueous solution, extraction of organic species from the aqueous and nonaqueous media.

Chromatography: Classification, principle and efficiency of the technique.

Mechanism of separation: adsorption, partition & ion exchange.

Development of chromatograms: frontal, elution and displacement methods.

Qualitative and quantitative aspects of chromatographic methods of analysis: IC, GLC, GPC, TLC and HPLC.

Stereoisomeric separation and analysis: Measurement of optical rotation.

(10 Lectures)

Reference Books:

• Mendham, J., *A. I. Vogel's Quantitative Chemical Analysis 6th Ed.,* Pearson, 2009.
• Willard, H.H. *et al.*: *Instrumental Methods of Analysis*, 7th Ed. Wardsworth Publishing Company, Belmont, California, USA, 1988.
• Christian, G.D. *Analytical Chemistry*, 6th Ed. John Wiley & Sons, New York, 2004.
• Harris, D.C.: *Exploring Chemical Analysis*, 9th Ed. New York, W.H. Freeman, 2016.
• Khopkar, S.M. *Basic Concepts of Analytical Chemistry*. New Age International Publisher, 2009.
• Skoog, D.A. Holler F.J. & Nieman, T.A. *Principles of Instrumental Analysis*, Cengage Learning India Ed.
• Mikes, O. *Laboratory Hand Book of Chromatographic & Allied Methods*, Elles Harwood Series on Analytical Chemistry, John Wiley & Sons, 1979.
• Ditts, R.V. Analytical Chemistry; Methods of separation, van Nostrand, 1974.

DSE LAB: ANALYTICAL METHODS IN CHEMISTRY

(Credits: Practicals-02, 60 Lectures, Full Marks: 30)

I. Separation Techniques

1. Chromatography:

(a) Separation of mixtures (any one)

(i) Paper chromatographic separation of Fe^{3+}, Al^{3+}, and Cr^{3+}.

(ii) Separation and identification of the monosaccharides present in the given mixture (glucose & fructose) by paper chromatography. Reporting the Rf values.

(b) (i) Separate a mixture of Sudan yellow and Sudan Red by TLC technique and identify them on the basis of their Rf values (any one).

(ii) Chromatographic separation of the active ingredients of plants, flowers and juices by TLC

II. Solvent Extractions:

To separate a mixture of Ni^{2+} & Fe^{2+}

by complexation with DMG and extracting the Ni^{2+}- DMG complex in chloroform, and determine its concentration by spectrophotometry.

3. Determine the pH of the given aerated drinks fruit juices, shampoos and soaps.

4. Analysis of soil:

(i) Determination of pH of soil.

(ii) Total soluble salt

(iii) Estimation of calcium, magnesium, phosphate, nitrate

6. Ion exchange (any one):

(i) Determination of exchange capacity of cation exchange resins and anion exchange resins.

(ii) Separation of metal ions from their binary mixture.

(iii) Separation of amino acids from organic acids by ion exchange chromatography.

III Spectrophotometry (any three)

1. Determination of pKa values of indicator using spectrophotometry.

2. Structural characterization of compounds by infrared spectroscopy.

3. Determination of dissolved oxygen in water.

4. Determination of chemical oxygen demand (COD).

5. Determine the composition of the Ferric-salicylate/ ferric-thiocyanate complex by Job's method.

Reference Books:

• Mendham, J., *A. I. Vogel's Quantitative Chemical Analysis 6th Ed.,* Pearson, 2009.
• Willard, H.H. *et al.*: *Instrumental Methods of Analysis*, 7th Ed. Wardsworth Publishing Company, Belmont, California, USA, 1988.
• Christian, G.D. *Analytical Chemistry*, 6th Ed. John Wiley & Sons, New York, 2004.
• Harris, D.C. *Exploring Chemical Analysis,* 9th Ed. New York, W.H. Freeman, 2016.
• Khopkar, S.M. *Basic Concepts of Analytical Chemistry*. New Age International Publisher, 2009.
• Skoog, D.A. Holler F.J. and Nieman, T.A. *Principles of Instrumental Analysis*, Cengage Learning India Edition.
• Mikes, O. & Chalmes, R.A. *Laboratory Handbook of Chromatographic & Allied Methods*, Elles Harwood Ltd. London.
• Ditts, R.V. *Analytical Chemistry: Methods of separation.* Van Nostrand, New York, 1974.

Semester VI

CHEM06C13: INORGANIC CHEMISTRY-IV

(Credits: Theory-04, 60 Lectures, Full Marks: 70)

Theoretical Principles in Qualitative Analysis (H_2S Scheme)

Basic principles involved in analysis of cations and anions and solubility products, common ion effect. Principles involved in separation of cations into groups and choice of group reagents. Interfering anions (fluoride, borate, oxalate and phosphate) and need to remove them after Group II.

(10 Lectures)

Organometallic Compounds

Definition and classification of organometallic compounds on the basis of bond type.

Concept of hapticity of organic ligands. Metal carbonyls: 18 electron rule, electron count of mononuclear, polynuclear and substituted metal carbonyls of 3d series. General methods of preparation (direct combination, reductive carbonylation, thermal and photochemical decomposition) of mono and binuclear carbonyls of 3d series. Structures of mononuclear and binuclear carbonyls of Cr, Mn, Fe, Co and Ni using VBT. π-acceptor behaviour of CO (MO diagram of CO to be discussed), synergic effect and use of IR data to explain extent of back bonding. Zeise's salt: Preparation and structure, evidences of synergic effect and comparison of synergic effect with that in carbonyls. Metal Alkyls: Important structural features of methyl lithium (tetramer) and trialkyl aluminium (dimer), concept of multicentre bonding in these compounds. Role of triethylaluminium in polymerisation of ethene (Ziegler – Natta Catalyst). Species present in ether solution of Grignard reagent and their structures, Schlenk equilibrium.

Ferrocene: Preparation and reactions (acetylation, alkylation, metallation, Mannich Condensation). Structure and aromaticity. Comparison of aromaticity and reactivity with that of benzene. **(30 Lectures)**

Reaction Kinetics and Mechanism

Introduction to inorganic reaction mechanisms. Substitution reactions in square planar complexes, Trans- effect, theories of trans effect, Mechanism of nucleophilic substitution in square planar complexes, Thermodynamic and Kinetic stability, Kinetics of octahedral substitution, Ligand field effects and reaction rates, Mechanism of substitution in octahedral complexes. **(10 Lectures)**

Catalysis by Organometallic Compounds

Study of the following industrial processes and their mechanism:

1. Alkene hydrogenation (Wilkinson's Catalyst)
2. Hydroformylation (Co salts)

3. Wacker Process

4. Synthetic gasoline (Fischer Tropsch reaction)

5. Synthesis gas by metal carbonyl complexes **(10 Lectures)**

Reference Books:

- Svehla, G. Vogel's Qualitative Inorganic Analysis, 7th Edition, Prentice Hall, 1996.
- Cotton, F.A.G.; Wilkinson & Gaus, P.L. Basic Inorganic Chemistry 3rd Ed.; Wiley India,
- Huheey, J. E.; Keiter, E.A. & Keiter, R.L. Inorganic Chemistry, Principles of Structure and Reactivity 4th Ed., Harper Collins 1993, Pearson,2006.
- Sharpe, A.G. Inorganic Chemistry, 4th Indian Reprint (Pearson Education) 2005
- Douglas, B. E.; McDaniel, D.H. & Alexander, J.J. Concepts and Models in Inorganic Chemistry3rd Ed., John Wiley and Sons, NY, 1994.
- Greenwood, N.N. & Earnshaw, A. Chemistry of the Elements, Elsevier 2nd Ed, 1997 (Ziegler Natta Catalyst and Equilibria in Grignard Solution).
- Lee, J.D. Concise Inorganic Chemistry 5th Ed., John Wiley and sons 2008.
- Powell, P. Principles of Organometallic Chemistry, Chapman and Hall, 1988.
- Shriver, D.D. & P. Atkins, Inorganic Chemistry 2nd Ed., Oxford University Press, 1994.
- Basolo, F. & Pearson, R. Mechanisms of Inorganic Reactions: Study of Metal Complexes in Solution 2nd Ed., John Wiley & Sons Inc; NY.
- Purcell, K.F. & Kotz, J.C., Inorganic Chemistry, W.B. Saunders Co. 1977
- Miessler, G. L. & Tarr, D.A. Inorganic Chemistry 4th Ed., Pearson, 2010.
- Collman, J. P. et al. Principles and Applications of Organotransition Metal Chemistry. Mill Valley, CA: University Science Books, 1987.
- Crabtree, R. H. The Organometallic Chemistry of the Transition Metals. j New York, NY: John Wiley, 2000.
- Spessard, G. O. & Miessler, G.L. Organometallic Chemistry. Upper Saddle River, NJ: Prentice-Hall, 1996.

CHEMISTRY PRACTICAL-C13 LAB

(Credits: Practicals-02, 60 Lectures, Full Marks: 30)

Cation radicals derived from:

Na, K, NH_3, Mg, Ca, Sr, Ba, Al, Pb, Bi, Cr, Mn, Fe, Co, Ni, Cu, Zn, Cd

Anion radicals:

F^-, Cl^-, Br^-, I^-, NO_3^-, NO_2^-, SCN^-, S^{2-}, SO_4^{2-}, $S_2O_3^{2-}$, PO_4^{3-}, BO_3^{3-}, CrO_4^{2-}, BrO_3^-, IO_3^-, $[Fe(CN)_6]^{4-}$, $[Fe(CN)_6]^{3-}$

Detection and confirmation of four radicals by macro, semi- micro tests and assignment of probable composition of the mixtures.

Mixtures should preferably contain one interfering anion, or insoluble component ($BaSO_4$,

$SrSO_4$, $PbSO_4$, CaF_2 or Al_2O_3) or combination of anions

Spot tests should be done whenever possible.

Any two of the followings:

(i). Measurement of 10 Dq by spectrophotometric method

(ii). Verification of spectrochemical series.

(iii). Controlled synthesis of two copper oxalate hydrate complexes: kinetic vs thermodynamic factors.

(iv). Preparation of acetylacetanato complexes of Cu^{2+}/Fe^{3+}. Find the λ_{max} of the complex.

(v). Synthesis of ammine complexes of Ni(II) and its ligand exchange reactions (e.g. bidentate ligands like acetylacetone, DMG, glycine) by substitution method.

Reference Books

- Vogel's Qualitative Inorganic Analysis, Revised by G. Svehla. Pearson Education, 2002.
- Marr & Rockett Practical Inorganic Chemistry. John Wiley & Sons 1972.

CHEM06C14: ORGANIC CHEMISTRY-V

(Credits: Theory-04, 60 Lectures, Full Marks: 70)

Organic Spectroscopy

General principles Introduction to absorption and emission spectroscopy.

UV Spectroscopy: Types of electronic transitions, λ_{max}, Chromophores and Auxochromes, Bathochromic and Hypsochromic shifts, Intensity of absorption; Application of Woodward Rules for calculation of λ_{max} for the following systems: α,β unsaturated aldehydes, ketones, carboxylic acids and esters; Conjugated dienes: alicyclic, homoannular and heteroannular; Extended conjugated systems (aldehydes, ketones and dienes); distinction between *cis* and *trans* isomers.

IR Spectroscopy: Fundamental and non-fundamental molecular vibrations; IR absorption positions of O, N and S containing functional groups; Effect of H-bonding, conjugation, resonance and ring size on IR absorptions; Fingerprint region and its significance; application in functional group analysis.

NMR Spectroscopy: Basic principles of Proton Magnetic Resonance, chemical shift and factors influencing it; Spin–Spin coupling and coupling constant; Anisotropic effects in alkene, alkyne, aldehydes and aromatics, Interpretation of NMR spectra of simple compounds.

Applications of IR, UV and NMR for identification of simple organic molecules. **(24 Lectures)**

Carbohydrates

Occurrence, classification and their biological importance.

Monosaccharides: Constitution and absolute configuration of glucose and fructose, epimers and anomers, mutarotation, determination of ring size of glucose and fructose, Haworth projections and conformational structures; Interconversions of aldoses and ketoses; Kiliani- Fischer synthesis and Ruff degradation;

Disaccharides – Structure elucidation of maltose, lactose and sucrose.

Polysaccharides – Elementary treatment of starch, cellulose and glycogen. **(16 Lectures)**

Dyes

Classification, Colour and constitution; Mordant and Vat Dyes; Chemistry of dyeing; Synthesis and applications of: Azo dyes-Methyl Orange and Congo Red (mechanism of Diazo Coupling); Triphenyl Methane Dyes-Malachite Green, Rosaniline and Crystal Violet; Phthalein Dyes – Phenolphthalein and Fluorescein; Natural dyes –structure elucidation and synthesis of Alizarin and Indigotin; Edible Dyes with examples.

(8 Lectures)

Polymers

Introduction and classification including di-block, tri-block and amphiphilic polymers; Number average molecular weight, Weight average molecular weight, Degree of polymerization, Polydispersity Index.

Polymerisation reactions -Addition and condensation -Mechanism of cationic, anionic and free radical addition polymerization; Metallocene-based Ziegler-Natta polymerisation of alkenes; Preparation and applications of plastics – thermosetting (phenol-formaldehyde, Polyurethanes) and thermosoftening (PVC, polythene);

Fabrics – natural and synthetic (acrylic, polyamido, polyester); Rubbers – natural and synthetic: Buna-S, Chloroprene and Neoprene; Vulcanization; Polymer additives; Introduction to liquid crystal polymers; Biodegradable and conducting polymers with examples.

(12 Lectures)

Reference Books:

- Kalsi, P. S. Textbook of Organic Chemistry 1st Ed., New Age International (P) Ltd. Pub.
- Morrison, R. T. & Boyd, R. N. Organic Chemistry, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- Billmeyer, F. W. Textbook of Polymer Science, John Wiley & Sons, Inc.
- Gowariker, V. R.; Viswanathan, N. V. & Sreedhar, J. Polymer Science, New Age International (P) Ltd. Pub.
- Finar, I. L. Organic Chemistry (Volume 2: Stereochemistry and the Chemistry of Natural Products), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
- Graham Solomons, T.W. Organic Chemistry, John Wiley & Sons, Inc.
- McMurry, J.E. Fundamentals of Organic Chemistry, 7th Ed. Cengage Learning India Edition, 2013.
- Clayden, J.; Greeves, N.; Warren, S.; Wothers, P.; Organic Chemistry, Oxford University Press.
- Singh, J.; Ali, S.M. & Singh, J. Natural Product Chemistry, Prajati Prakashan

(2010).
- Kemp, W. Organic Spectroscopy, Palgrave.
- Pavia, D. L. et al. Introduction to Spectroscopy 5th Ed. Cengage Learning India Ed. (2015).

CHEMISTRY PRACTICAL-C14 LAB

(Credits: Practicals-02, 60 Lectures, Full Marks: 30)

1. Extraction of caffeine from tea leaves.
2. Preparation of sodium polyacrylate.
3. Preparation of urea formaldehyde.
4. Analysis of Carbohydrate: aldoses and ketoses, reducing and non-reducing sugars.
5. Qualitative analysis of unknown organic compounds containing monofunctional groups (carbohydrates, aryl halides, aromatic hydrocarbons, nitro compounds, amines and amides) and simple bifunctional groups, for *e.g.* salicylic acid, cinnamic acid, nitrophenols, etc.
6. Identification of simple organic compounds by IR spectroscopy and NMR spectroscopy (Spectra to be provided).
7. Preparation of methyl orange.

Reference Books:

- Vogel, A.I. Quantitative Organic Analysis, Part 3, Pearson (2012).
- Mann, F.G. & Saunders, B.C. Practical Organic Chemistry, Pearson Education (2009)
- Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. Practical Organic Chemistry, 5th Ed., Pearson (2012)
- Ahluwalia, V.K. & Aggarwal, R. Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis, University Press (2000).
- Ahluwalia, V.K. & Dhingra, S. Comprehensive Practical Organic Chemistry: Qualitative Analysis, University Press (2000).

CHEMISTRY-DSE 3 and 4 (ELECTIVES)

Credit: 4 + 2

CHEM06DSE:

7. FLUORESCENCE STUDY FOR THE SENSING AND MACROMOLECULAR INTERACTIONS

(Credits: Theory-04, 60 Lectures, Full Marks: 70)

Basic idea of spectral intensities: Fermi Golden rule and selection rules from quantum mechanical view points.

Potential energy curves, mirror-image symmetry, deactivation – internal conversion and intersystem crossing, radiationless deactivation, Quenching of fluorescence, Stern-Volmer equation and plot, static and dynamic quenching, Life-time variation in presence of quencher. Fluorescence quenching study of tryptophan in protein for the sensing of organic molecules, partial accessibility of tryptophan – modified Stern Volmer plot, study of different folding states. Protein – surfactant interaction, protein – polymer interaction and protein – DNA interaction.

Excimers and exciplexes. Intermolecular energy transfer (FRET). Energy transfer and conformation distributions of biopolymers.

Principles of LASER and characteristic features.

Preliminary ideas of absorption and fluorescence spectrophotometer. Basic ideas of dynamics namely TCSPC, up-conversion and pump-probe techniques.

Reference Book:

Principles of Fluorescence Spectroscopy, 3rd edition, Joseph R. Lakowicz.

DSE LAB: FLUORESCENCE STUDY FOR THE SENSING AND MACROMOLECULAR INTERACTIONS

(Credits: Practicals-02, 60 Lectures, Full Marks: 30)

1. Fluorescence quenching of organic fluorophores
2. Fluorescence quenching of tryptophan in different folding states of protein
3. Sensing of organic molecules by protein fluorescence study
4. FRET for suitable donor – acceptor pair
5. Protein fluorescence in presence of surfactants, polymers

8. Seminar / Review / Grand Viva

(Credits: Theory-04, Practicals-02, Full Marks-100)

9. RETROSYNTHESIS AND STRATEGY FOR ORGANIC SYNTHESIS

(Credits: Theory-04, 60 Lectures, Full Marks: 70)

Synthetic strategy:

Retrosynthetic analysis- disconnections, synthons, donor and acceptor synthons, functional group interconversion, C-C disconnections and synthesis [one group and two group (1,2 to 1,6-dioxygenated)], reconnection (1,6-di carbonyl), natural reactivity and umpolung, protection-deprotection strategy [alcohol, amine, carbonyl, acid]. **(14 Lectures)**

Asymmetric synthesis:

Stereoselective and stereospecific reactions, diastereoselectivity, and enantioselectivity (only definition), diastereoselectivity: addition of nucleophiles to C=O, adjacent to a stereogenic centre (Felkin-Anh model); addition of electrophiles to C=C (Houk model). **(12 Lectures)**

Carbocycles:

Synthesis and reactions: Thermodynamic and kinetic factors, Baldwin rules. Synthesis of carbocycles through alkylation, condensation, cycloaddition, rearrangement and their reactions. Synthesis of polycyclic aromatics. **(8 Lectures)**

Organometallic Chemistry:

Preparation and Application of organo-Si, Cd, Se, Ti, Pd *etc*. **(8 Lectures)**

Pericyclic Reactions:

Electrocyclic reactions: 4e and 6e neutral systems; cycloaddition reactions: [4 + 2] and [2 + 2] reactions, cheletropic addition of carbene; sigmatropic rearrangements: [1,3] and [1,5] H shifts, [3,3] Cope and Claisen rearrangements. FMO analysis and Woodward-Hoffmann selection rules.

(18 Lectures)

Reference Book

Organic Synthesis: The Disconnection Approach by Stuart Warren, Publisher: Wiley

DSE LAB: RETROSYNTHESIS AND STRATEGY FOR ORGANIC SYNTHESIS

(Credits: 02, 60 Lectures, Full Marks: 30)

1. Preparation of organic molecules using Grignard reagent
2. Aldol condensation
3. Michael reaction
4. Esterification reaction
4. Diel-Alder reaction

Structure and Detailed Syllabus of the Postgraduate Course (M.Sc.) in Chemistry
Department of Chemistry
Presidency University

(Effective from Academic Year 2022-23)

PRESIDENCY UNIVERSITY
KOLKATA

Department of Chemistry

(Faculty of Natural and Mathematical Sciences)
Presidency University
Hindoo College (1817-1855), Presidency College (1855-2010)
86/1, College Street, Kolkata - 700 073
West Bengal, India

Aim of the Programme / Programme Outcomes:

1. Create an amicable learning environment among students to inculcate the deep interests and knowledge in subject.
2. Provide choice-based learning in specific sub discipline of chemistry.
3. Help students to develop the ability to use their knowledge and skills to interpret and handle the problem arises in day-to-day life.
4. Motivate students to pursue advanced studies on their subject of interest in the industry, academics and research institutions of repute.
5. Educate and enhancing student generic skills through skill enhancement courses, lab based, value added and project-based courses, this may help them creating employment and business opportunities in academia and industries.

Programme specific learning outcomes

A graduating student of M.Sc. Chemistry degree expected to:

1. Have proficient theoretical and experimental knowledge in the broad subject area of chemistry as well as different sub-fields of chemistry such as Analytical Chemistry, Inorganic Chemistry, Organic Chemistry, Physical Chemistry, Material Chemistry, etc.
2. Explain, integrate and apply the acquired knowledge to problems that are emerging from the interdisciplinary areas.
3. Be aware of current developments at the forefront in Chemistry and allied subjects.
4. Have hands-on training on various analytical techniques, classical qualitative and quantitative chemical analysis, which enables their job opportunity on chemical industries and various nationalized analytical labs.
5. Have knowledge on hazardous chemical, safe handling of chemicals and role of chemistry on environmental issues.
6. Carry out experiments independently as well as be able to work productively in groups.
7. Construct a research problem as per the social requirement.
8. Communicate the scientific work in oral, written and e- formats as per the requirements.

Structure of Postgraduate Chemistry Course

<table>
<tr><th rowspan="3">Semester</th><th colspan="7">Course Description with Marks</th></tr>
<tr><th colspan="6">Theory</th><th rowspan="2">Lab</th></tr>
<tr><th>Organic Chemistry</th><th>Inorganic Chemistry</th><th>Physical Chemistry</th><th>Common Paper</th><th>Special Paper (Organic/Inorganic /Physical)</th><th>Total</th></tr>
<tr><td>First</td><td>50
(CHEM 0701)</td><td>50
(CHEM 0702)</td><td>50
(CHEM 0703)</td><td>-</td><td>-</td><td>150</td><td>Inorganic Lab: 50
(CHEM 0791)
Physical Lab: 50
(CHEM 0792)</td></tr>
<tr><td>Second</td><td>50
(CHEM 0801)</td><td>50
(CHEM 0802)</td><td>50
(CHEM 0803)</td><td>-</td><td>-</td><td>150</td><td>Organic Lab: 50
(CHEM 0891)
Computer Application: 50
(CHEM 0892)</td></tr>
<tr><td rowspan="3">Third</td><td rowspan="2">-</td><td rowspan="2">-</td><td rowspan="2">-</td><td>50
(CHEM 0901)</td><td>-</td><td rowspan="3">150</td><td rowspan="3">Advanced Organic /Inorganic/Physical Lab: 50
(CHEM 0991A/B/C)
Research Based Lab: 50
(CHEM 0992)</td></tr>
<tr><td>50
(CHEM 0902)</td><td>-</td></tr>
<tr><td>-</td><td>-</td><td>-</td><td>-</td><td>50
(CHEM 0903A/B/C)</td></tr>
<tr><td rowspan="3">Fourth</td><td rowspan="3">-</td><td rowspan="3">-</td><td rowspan="3">-</td><td rowspan="3">-</td><td>50
(CHEM 1001A/B/C)</td><td rowspan="2">100</td><td rowspan="3">Project Work
(CHEM 1091 and CHEM 1092):
50 + 50</td></tr>
<tr><td>50
(CHEM 1002A/B/C)</td></tr>
<tr><td>50 (CHEM 1003)
Seminar/Review and Grand Viva</td><td>50</td></tr>
<tr><td colspan="7">600</td><td>400</td></tr>
</table>

Course Structure for two-year M.Sc. Programme in Chemistry (with effect from the academic session 2022-23) Semester-wise distribution of Courses

Semester	Paper Code	Name of the Courses	Full Marks	Credit Points	Course type†
1	**CHEM 0701**	General Organic Chemistry - I	50 (35 + 15)	4	T
	CHEM 0702	General Inorganic Chemistry – I	50 (35 + 15)	4	T
	CHEM 0703	General Physical Chemistry - I	50 (35 + 15)	4	T
	CHEM 0791	Inorganic Chemistry Lab	50	4	P, S
	CHEM 0792	Physical Chemistry Lab	50	4	P, S
		Total	**250**	**20**	
2	**CHEM 0801**	General Organic Chemistry - II	50 (35 + 15)	4	T
	CHEM 0802	General Inorganic Chemistry – II	50 (35 + 15)	4	T
	CHEM 0803	General Physical Chemistry - II	50 (35 + 15)	4	T
	CHEM 0891	Organic Chemistry Lab	50	4	P, S
	CHEM 0892	Computer Application	50	4	P, S
		Total	**250**	**20**	
3	**CHEM 0901**	Symmetry, Macromolecules and Magnetic Resonance	50 (35 + 15)	4	T
	CHEM 0902	Spectroscopy, Supramolecules and Nanomaterials	50 (35 + 15)	4	T
	CHEM 0903	Advanced Organic/Inorganic/Physical Chemistry -I *	50 (35 + 15)	4	T
	CHEM 0991	Advanced Organic/Inorganic/Physical Chemistry Lab**	50	4	P, S
	CHEM 0992	Research Based Lab	50	4	P, S
		Total	**250**	**20**	
4	**CHEM 1001**	Advanced Organic/Inorganic/Physical Chemistry -II*	50 (35 + 15)	4	T
	CHEM 1002	Advanced Organic/Inorganic/Physical Chemistry -III *	50 (35 + 15)	4	T
	CHEM 1003	Seminar/Review and Grand Viva	50	4	S
	CHEM 1091	Project Dissertation	50	4	P, S
	CHEM 1092	Project presentation, defense, proposal	50	4	P, S
		Total	**250**	**20**	
		Grand Total	**1000**	**80**	

† In Course Type, 'T' stands for Theory, P stands for Practical and 'S' stands for Sessional papers.

* Based on the specialization, Advanced Organic/Inorganic/Physical Chemistry theory papers, namely, CHEM0903, CHEM1001 and CHEM1002 are offered (semester 3 and 4) from respective sections: three streams differentiating A – Organic chemistry, B – Inorganic chemistry, and C – Physical chemistry.

** Based on the specialization, Advanced Organic/Inorganic/Physical Chemistry Lab paper (CHEM0991) is offered (semester 3) from respective sections: three streams differentiating A – Organic chemistry, B – Inorganic chemistry, and C – Physical chemistry

The methods of assessments for Sessional papers are continuous evaluation throughout the semester

The theory paper marks 50 (35+15) indicates (End semester examination 35 + Internal Assessment 15)

FIRST SEMESTER

Course No. CHEM 0701 (FM = 50; C = 4)
General Organic Chemistry-I

Course Objectives: This course aims to impart advanced level knowledge on (i) conformational aspects of alicyclic compounds and its implication in organic synthesis; (ii) the concept of concerted reaction, MO & symmetry of polyenes in controlling the stereochemical outcome of the reaction and its application in organic synthesis (iii) Modern spectroscopic techniques used in chemistry and the structure elucidation of organic compounds (problem solving) based on these techniques.

Unit 1: Stereochemistry (M = 15)

Static Aspects: Symmetry properties, point group; configuration – acyclic and cyclic systems; conformation – cyclic systems (cyclohexene, cyclohexanone, substituted cyclopentanes and cyclopentanones, medium rings, decalin and hydrindane systems).

Dynamic Aspects: cyclisation reactions, Baldwin's Rules; conformation and reactivity with reference to substitution, elimination, addition and rearrangement reactions.

Unit 2: Pericyclic reactions (M = 18)

Pericyclic reactions: Molecular orbitals for acyclic conjugated systems. Theory of pericyclic reactions – i) Frontier Molecular Orbital (FMO) approach ii) concept of aromaticity of transition states (Hückel / Möbius systems). The Woodward-Hoffmann selection rules and general rules.

General perturbation molecular orbital theory in cycloadditions: Symmetry principles in pericyclic reactions, orbital and state correlation diagram for electrocyclic and cycloaddition reactions. Reactivity, regioselectivity and periselectivity. Cycloaddition reactions: antarafacial and suprafacial additions, 4n and 4n+2 systems; 2,2 addition of ketenes, 1,3 dipolar cycloadditions and cheleotropic reactions. Ene reactions, group-transfer reactions and eliminations. Scope, reactivity and stereochemical features of electrocyclic reactions (4e, 6e and 8e neutral systems). Electrocyclic reactions of charged systems (cations and anions), Electrocyclic reactions: conrotatory and disrotatory motions, 4n, 4n+2 and allyl systems.

Sigmatropic rearrangements: [1, j] shifts – [1, 5] and [1, 7] shifts in neutral systems and [1,4] shift in charged species: [i, j] shifts – [3, 3] shifts, Sommelet-Hauser, Cope, aza-Cope rearrangements, Fluxional tautomerism. Claisen rearrangements; [5, 5] shifts, [2, 3] shifts in ylids.

Unit 3: Spectroscopy (M = 17)

Review of UV and IR spectroscopy ^{1}H NMR Spectroscopy: Basic theory – phenomenon of energy absorptions (resonance) and relaxation, chemical shift, shielding and deshielding mechanisms, equivalence and nonequivalence of protons, spin-spin coupling – notation for spin systems, coupling constant and its variation with stereochemistry – Karplus equation. Structural application of ^{1}H NMR, aromaticity, antiaromaticity and homoaromaticity of organic molecules and related problems.

^{13}C NMR Spectroscopy: Principles; broad band decoupling, DEPT; structural applications of ^{13}C NMR.

Mass Spectrometry: Types of ionization techniques, basic principles of EI, fragmentation pattern of small molecules.

Problems incorporating spectroscopic data.

References:

1. Stereochemistry of Organic Compounds - E. L. Eliel and S. H. Wilen, Wiley India Ed, 2008.

2. Stereochemistry of Organic Compounds: Principles and Applications – D. Nassipuri, New Age International, 1994.

3. Advanced Organic Chemistry (Part A & B) - F.A. Carey and R. J. Sundberg,

Springer Science + Business Media, 5th Ed, 2007.
4. Organic Chemistry - J. Clayden, N. Greeves and S. Warren, Oxford University Press, 2nd Ed, 2012.
5. The Conservation of Orbital Symmetry - R.B. Woodward and R. Hoffmann, Academic Press, 1971
6. Organic Reactions and Orbital Symmetry - P. L. Gilchrist and R. C. Storr, Cambridge [Eng.] University Press, 1972.
7. Pericyclic Chemistry -Orbital Mechanisms and Stereochemistry -D. K. Mandal, Elsevier, 2018.
8. Pericyclic Reaction - I. Fleming, Oxford University Press, 1998.
9. Molecular Orbitals and Organic Chemical Reactions - I. Fleming, John Wiley and Sons, Ltd.
10. Orbital Symmetry- A Problem-Solving Approach – R. E. Lehr, Alan P. Marchand, Academic Press INC, 1972.
11. Pericyclic Reactions - A Text Book: Reactions, Applications and Theory – S. Sankararaman, Wiley-VCH, 2005
12. Organic Spectroscopy - W. Kemp, ELBS
13. Introduction to Spectroscopy - D. L. Pavia, G. M. Lampman, G. S. Kriz and J. R. Vyvyan, Cengage Learning India Pvt. Ltd.
14. Applications of Absorption Spectroscopy of Organic Compounds – J. R. Dyer, Prentice Hall India Learning Pvt. Ltd.
15. Spectrometric Identification of Organic Compounds by R. M. Silverstein and G. C. Bassler, and T. C. Morrill, Spectrometric identification of Organic compounds, John Wiley & Sons, 5th Ed, 1991
16. Spectrometric method in Organic Chemistry - D.H. Williams and I. Fleming, Tata McGraw Hill Education.
17. NMR Spectroscopy: Basic Principle, Concepts and Applications in Chemistry - H. Günther, Wiley
18. Organic Structure Determination – J. H. Simpson, Elsevier
19. NMR Spectroscopy Explained – N. E Jacobsen, Wiley

Course Learning Outcomes: After completion of the course, the student should be able to

(i) Improve the basic idea of stereochemistry of organic compounds (small to large ring systems)

(ii) Analyze pericyclic reactions: Electrocyclic reactions, Sigmatropic Rearrangements and Cycloadditions and explain their feasibility in the light of

FMO approach.

(iii) Explain theoretical idea of nuclear magnetic spectroscopy (NMR), IR spectroscopy and Mass spectrometry to understand the spectra and characterize simple/complex organic molecules.

Course CHEM 0702 (FM = 50; C = 4)

General Inorganic Chemistry-I

Course Objectives: This course is designed to convey knowledge on basic and advanced level chemistry of coordination compounds, f-block compounds and Chemical equilibrium of inorganic complexes. Some special structural features of boranes and their industrial applications.

Unit 1 Coordination chemistry(I): Structure, stability and reactivity (M= 18)

Thermodynamic aspects of crystal field splitting, kinetics aspects of crystal field splitting, crystal field activation energy, labile and inert complexes. Single ion magnetic behavior, metal centered transitions.

Limitations of CFT, evidences of metal-ligand orbital overlap, nephelauxetic series; spectrochemical series. Free ion terms arising from d^n configuration and their splitting in Oh and Td fields – Orgel diagrams. Charge transfer spectra – LMCT and MLCT transition in O_h and T_d complexes.

Structural and stereoisomerism of coordination compounds, optically active coordination compounds and their resolution procedures, absolute configuration of enantiomers.

Unit 2 Chemistry of elements: Special features (M = 16)

Structure and bonding of higher boranes, carboranes, metallocarboranes, Lipscomb's tropological diagrams and Wade's rules. Metal Clusters (low and high nuclearity carbonyl clusters), Skeletal electron counting, Wade-Mingos rule, application of iso electronic and isolobal relationships and caping rules. Metal-metal bonded complexes of metals (structure and bonding): dirhenium complexes, transition metal dioxygen and dinitrogen complexes (structure, bonding and reactivity), Vaska's complex. Alkali metal complexes with macrocyclic ligands, crown ether and cryptate complexes.

Unit 3 Chemistry of f-block elements (M = 8)

Relativistic effect; Magnetic properties and electronic spectra of lanthanides and actinides; use of lanthanide compounds as NMR-shift reagent and MRI-contrast agent; Super heavy elements

Unit 4 Chemistry of Complex Equilibria (M = 8)

Kinetic-, thermodynamic stability of metal complexes. Statistical and non-statistical factors influencing stability of complexes in solution, stability and reactivity of mixed ligand complexes. Determination of composition and stability constants of complexes by pH metric, spectrophotometric and polarographic methods. Solubility Equilibria – quantitativeness of precipitation (of metal hydroxides, sulphides and chelates).

References:

1. The f Elements - Nikolas Kaltsoyannis and Peter Scott
2. Concepts and Models of Inorganic Chemistry - Douglas, B.E. and McDaniel, D.H.
3. Inorganic Chemistry, Principles of Structure and Reactivity 4th Ed. - Huheey, J. E.; Keiter, E.A. & Keiter, R.L.
4. B.N. Figgies: Ligand Field Theory and its Applications General and Inorganic Chemistry: R. P. Sarkar, Vol II
5. Inorganic chemistry - Keith F. Purcell, John C. Kotz.
6. Multiple Bonds between Metal Atoms - Carlos A. Murillo, F. Albert Cotton, Richard A Walton, Richard A. Walton.
7. Inorganic Chemistry - Duward Shriver, Mark Weller, Tina Overton, Jonathan Rourke, Fraser Armstrong
8. Selected Topics in Inorganic Chemistry - W. U. Malik, G. D. Tuli, R. D. Madan.

Course Learning Outcomes: After the completion of the course, the students should be able to

1. Explain the origin of color using various theoretical phenomenon such as Orgel and Tanabe-Sugano diagram.
2. Explain the color intensity, reason of different color, reason of existence of

magnetism etc.
3. Explain lanthanide-based NMR-shift and MRI contrast reagent.
4. Determine the chemical composition and ligand lability properties using different techniques.
5. Structure and bonding of boranes using Lipscomb topological approach, Wade's rule and isolobal analogy.

Course No. CHEM 0703 (FM = 50; C = 4)
General Physical Chemistry-I

Course Objectives: To provide basic knowledge of molecular spectroscopy, partition function, ionic atmosphere and collision theory.

Unit 1 Molecular Spectroscopy (M=14)

Molecular spectroscopy: Introduction, elementary idea about spectroscopic instrumentation, spectral broadening. Electromagnetic spectrum and molecular processes associated with the regions. Rotational spectra of polyatomic molecules: classification of molecules into spherical, symmetric and asymmetric tops; linear triatomic molecules, Non-rigid rotor. Elementary idea of Stark effect. Anharmonic oscillator and dissociation. Elementary idea of Born-Oppenheimer approximation. Vibration rotation spectra for diatomic molecule, Rotational-vibrational coupling. Raman spectra: classical theory of Raman scattering, concept of polarizability ellipsoid.

Unit 2 Statistical mechanics- l (M = 12)

Probability, thermodynamic probability and entropy, Maxwell-Boltzman statistics, Partition function: translational (for ideal gas - concept of thermal wavelength), rotational, vibrational and electronic partition functions (diatomic molecule); molecular and molar partition function, Qualitative idea of Quantum statistics (Bose-Einstein, Fermi-Dirac statistics): Thermodynamic probability and distribution formula (without derivation), comparison with classical statistics - distinguishability and indistinguishability of identical particles.

Application: Theory of specific heat of solids – Einstein's and Debye's pictures.

Unit 3 Electrochemistry (M = 09)

Debye-Hückel theory of strong electrolytes, concept of ionic atmosphere. Debye-Hückel limiting law for single ionic activity coefficient and mean activity coefficient (with derivation), its relation to ionic strength. Bjerrum model for ion association: Formation of ion pairs, derivation of ion- association constant.

Unit 4 Kinetics-l (M = 15)

Collision theory: Lines of centre model. Introduction of potential energy surface and contour, internal coordinates and reaction coordinates, reaction path – valley and saddle point; saddle point – activation energy, classical trajectory, and theory of absolute rate. Comparison of collision and absolute rate theory. Fast reaction - relaxation methods. Branching chain reactions and explosion. Oscillatory reactions: Lotka-Volterra model and its applications.

Rate equation for electrode process. Butler-Volmer equation, High Field approximation, Tafel equation, Low field approximation, kinetic derivation of Nernst equation, exchange current density and polarizability of interfaces, concept of overvoltage. Kinetics of adsorption on solid, the adsorption isotherms (Langmuir, BET – with derivation)

References

1. Introduction to Atomic Spectra - White Harvey Elliott
2. Fundamentals of Molecular Spectroscopy - Banwell, C. N. & McCash, E. M.
3. Atomic Physics - Rajam J. B.
4. Introduction to Molecular Spectroscopy - Gordon M. Barrow
5. An Introduction to Statistical Thermodynamics - T. L. Hill
6. Statistical Mechanics - D. A. McQuarrie
7. Modern Electrochemistry 1: Ionics - J.O.M. Bockris; A.K.N. Reddy
8. An Introduction to Electrochemistry - S. Glasstone
9. Textbook of Physical Chemistry - S. Glasstone
10. Chemical Kinetics - Keith J. Laidler
11. Physical Chemistry - K.L. Kapoor
12. Physical Chemistry - Ashish K. Nag
13. Physical Chemistry - Gilbert W. Castellan

Course learning outcomes: After the completion of the course, the students should be able to

1. Explain the fundamentals of rotational, vibrational spectroscopy, introduction of anharmonicity, basics of spectroscopic instrumentation of and spectra for polyatomic molecules and concept of polarizability in Raman scattering.
2. Explain the concept of thermodynamic probability, its relation with absolute entropy and express different thermodynamic energy parameters in terms of partition functions and Einstein's and Debye's pictures for specific heat of solids.
3. Describe the activity coefficients of electrolyte solution as a function of concentration.
4. Evaluate the ion-association constants of in solutions of weak electrolytes, and estimate the extent of associated ions.
5. Explain the difference between collision and absolute rate theory, kinetics of branching reaction, charge transfer process for electrode reaction and multilayer adsorption phenomena.

Course No. CHEM 0791 (FM = 50; C =4)
Inorganic Chemistry Lab

Course Objectives: The course aims to provide practical skill on estimation of inorganic ions using colorimetry, physiochemical methods and Quantitative estimation of ions in real life sample like milk and cola etc.

PART 1

Quantitative estimation of inorganic ions by colorimetry (any one).

Colorimetric determination of 1) Fe^{3+} as sulphosalicylate complex 2) Fe^{2+} as phenanthroline complex 3)Manganese as MnO_4^- 4) Chromium as dichromate.

Physicochemical Experiments:

i) Determination of composition of complexes by continuous variation/ Mole- Ratio / Slope ratio method of the following systems: Fe (III) – sulphosalicylate complex; Fe (II) - phenanthroline complex

ii) A colorimetric study of the kinetics on inorganic reaction.

Part II (any two)

1. Determination of the amount of calcium in milk powder by EDTA complexometry
2. Potassium trioxaltoferrate III: Sythesis, analysis and photochemistry.
3. Analysis of kidney stones by permanganometric titration
4. Preparation of $[Ni(NH_3)6]^{2+}$ and its analysis by different methods
5. Estimation of iodine in iodized common salt using iodometry
6. Estimation of phosphoric acid in cola drinks by molybdenum blue method
7. Paper and column chromatography of plant pigments

References:

1. A. J. Elias, A Collection of Interesting General Chemistry Experiments, Sangam books
2. G. N. Mukherjee, Advanced Experiments in Inorganic Chemistry, U. N. Dhur & Sons(p) ltd.

Course Learning Outcomes: On completion of the course, the students should be able to

1. Estimate the various ions practically using colorimetric technique.
2. Estimate the various ions such as calcium, magnesium, phosphates, etc., present in real life day to day samples

Course No. CHEM 0792 (FM = 50; C = 4)
Physical Chemistry Lab

Course Objectives: To provide hand-on experiences of techniques for verifying physical and chemical properties and data interpretation skill.

1. Spectrophotometric experiment - determination of composition of a complex (Job's method)
2. Spectrophotometric experiment - Determination isosbestic point and indicator constant
3. Determination of cmc of surfactants: conductometry.
4. Determination of standard reduction potential of quinhydrone electrode.
5. Potentiometric determination of strength of halide mixture.
6. Determination of hydrolysis constant of NH_4Cl

7. Determination of molecular weight of macromolecules by viscometry.

Course learning outcomes: The students will acquire skills to

1. Handle instruments such as conductometer, potentiometer, spectrophotometer, viscometer, pH meter etc.
2. Analyze the data obtained from the experiments to measure various physico-chemical properties.

SECOND SEMESTER

Course No. CHEM 0801 (FM = 50; C = 4)

General Organic Chemistry-II

Course Objectives: This course aims to impart advanced level knowledge on (i) application of modern B, S, P and Si-based reagents in multistep organic synthesis (ii) designing synthetic strategies towards complex molecular targets such as bioactive heterocyclics and natural products including alkaloids, terpenoids and their structure elucidation.

Unit 1: Synthetic methodology and Synthetic strategy (M = 17)

Synthetic methodology: The roles of boron, phosphorus, sulfur and silicon in organic synthesis. Stereoselective hydroboration, hydrogenation, epoxidation and hydroxylation. Application of modern reagents in organic synthesis.

Synthetic strategy: Retrosynthetic analysis, disconnection, typical examples to illustrate the disconnection approach to organic synthesis.

Unit 2: Heterocyclic Chemistry (M = 17)

Systematic nomenclature (Hantzsch – Widman system) for monocycle and fused heterocycles.

General approach to heterocyclic synthesis – cyclisation and cycloaddition routes. Heterocycles in organic synthesis – masked functionalities, umpolung, Stork annulation reaction and applications (synthesis of testosterone, estrone, progesterone, ranitidine, lansoprazole and/or recently discovered molecules etc. Rearrangement and ring transformation involving 5- and 6-membered heterocycles with one heteroatom.

Unit 3: Natural products (M = 16)

Structural types; structure elucidation, reactions and synthesis of representative examples of (i) Alkaloids (ii) Terpenoids. Stereochemistry, reactions and synthesis of terpenoids and carotenoids: zingiberine, santonin, abietic acid, β-carotene. Stereochemistry, reactions and synthesis of alkaloids: quinine, morphine, camptothecin and recently discovered bioactive natural products.

References:

1. Modern Methods of Organic Synthesis - W. Carruthers, I. Coldham, CUP
2. Organic Chemistry - J. Clayden, N. Greeves, S. Warren and P. Wothers, OUP
3. Principle of Organic Synthesis - R.O.C. Norman and J.M. Coxon, Blackie

4. Organic Synthesis: The Disconnection Approach - S. Warren, Wiley
5. Organic Synthesis - M.B. Smith, McGraw - Hill
6. The Logic in Organic Synthesis - E.J. Corey and X. Cheng, Wiley
7. Organic Chemistry, Vol. II - I. L. Finar, ELBS
8. Mechanism and Theory in Organic Chemistry by Lowry and Richardson
9. Advanced Organic Chemistry: reactions, Mechanism and Structures (8th Edn) by J. March
10. Heterocycles in Organic Synthesis - A.I. Meyers, Wiley
11. Heterocyclic Chemistry - J.A. Joule and K. Mills, Blackwell
12. Heterocyclic Chemistry - T.L. Gilchrist, Wiley
13. Classics in Total Synthesis (Vol I) - K.C. Nicolaou and E.J. Sorensen, Wiley-VCH
14. Classics in Total Synthesis II - K.C. Nicolaou and S.A. Snyder Wiley-VCH

Course Learning Outcomes: After completion of the course, the student should be able to

1. Explicate the use of modern reagent and their chemistry based on boron, silicon, sulphur, phosphorus and retro synthesis of complex molecule.
2. Expand the knowledge of simple and complex organic molecules containing one or more heteroatom.
3. Elucidate structures, stereochemistry, a variety of total synthetic pathways and reactions of classical and recently discovered bioactive natural products (alkaloids, terpenoids and carotenoids).

Course No. CHEM 0802 (FM = 50; C = 4)

General Inorganic Chemistry-II

Course Objectives: Impart knowledge on the VBT and LCAO-MOT theory on diatomic hydrogen type molecule and show orbital overlap in pictorial representation. Familiarize students with organometallic clusters, cages and their catalytic application. To provide an introduction into symmetry of molecules.

Unit 1 Aspects of Chemical Bonding (M = 16)

Born-Oppenheimer Approximation, Valence bond theory (VBT), resonance in VBT, VBT of homonuclear diatomic molecules. Hybridization, participation of d orbitals in hybridization in polyatomic species. Molecular orbital theory (MOT), linear combination of atomic orbitals (LCAO), criteria for the formation of stable

MOs. LCAO-MO Treatment of diatomic hydrogen (H_2) and hydrogen molecule ion (H_2^+). Sigma, Pi and Delta molecular orbitals. MO of Homonuclear and heteronuclear diatomic molecules and ions. MO theory of polyatomic molecules and ions. Walsh diagram. MO theory of conjugated molecules. Combination of atomic orbitals (pictorial approach). MO concept of metal-ligand bonding (pictorial approach)

Unit 2 Organometallic Chemistry (M = 17)

Preliminary idea and applications of 16 and 18 electrons rule for organometallic compounds. Reaction of organometallic complexes: substitution, oxidative addition, reductive elimination, insertion and elimination, electrophilic and nucleophilic reactions of coordinated ligands. Stereochemical non-rigidity and fluxional behaviour of organometallic compounds, catalysis by organometallic compounds: CH functionalization reactions. Applications of organometallics in organic synthesis: C-C coupling reactions (Kumada, Negishi, Heck, Suzuki, Hiama and Stille reactions etc).C-N bond coupling reactions and asymmetric hydrogenations. Polymerization, oligomerization and metathesis reactions of alkenes and alkynes; Zieglar-Natta catalysis.

Unit 3 Principle of symmetry in Chemistry (M = 17)

Concept of symmetry in molecules, symmetry elements and symmetry operations, combining symmetry operations. Multiplication Table by stereographic projection technique. Elements of Group Theory, Sub groups and classes of group elements. Symmetry point groups of molecules, systematic classification of molecular point groups, Application of symmetry in identifying polar and chiral molecules. Symmetry and stereo-isomerism. Unit vector transformation and interpretation of character table. Matrix representation of symmetry, matrix diagonalizations, Construction of character table, reducible and irreducible representations. Identification of symmetry label of MO in a molecule. Construction of MO on the basis of Symmetry of the molecules (H_2O, NH_3, B_2H_6, CH_4). Two-dimensional space group.

References

1. Fundamental Concepts of Inorganic Chemistry (Vol. 2), ed. 2 - A. K. Das.
2. General and Inorganic Chemistry (Vol. 1) - R. P. Sarkar.
3. A Textbook of Physical Chemistry (Vol. 4) - K. L. Kapoor.

4. Symmetry and Spectroscopy of Molecules - K. V. Reddy.
5. Chemical Applications of Group Theory - F. A. Cotton.
6. Group Theory in Chemistry - A. K. Mukherjee, B. C. Ghosh.
7. Basic Organometallic Chemistry - A. Elias, B. D. Gupta.
8. Principles of Organometallic Chemistry - Powell, P.
9. The Organometallic Chemistry of the Transition Metals - Crabtree, R. H.

Course Learning Outcomes: On completion of the course, the students should be able to

1. Explain the concepts of VBT, and LCAO-MOT. The students should be able to represent orbital overlap diagram for sigma, pi- and delta bonding.
2. Explain the structures and electron counting schemes of organometallic compounds.
3. Demonstrate the structure and bonding, coordination modes, geometries, fundamental reaction types of organometallic compounds and the mechanisms in the organometallic catalytic processes.
4. Recognize symmetry elements in a molecule and deduce point group. Can represent matrices for symmetry representation.
5. Use character table to find out the symmetry labels for any orbitals and basis functions, which is extensively used in spectroscopy course. They will also be able to construct qualitative MOED diagram using character table.

Course No. CHEM 0803 (FM = 50; C = 4)
General Physical Chemistry-ll

Course Objectives: To impart basic knowledge of quantum mechanics, quantum numbers, atomic spectra and dielectric property.

Unit 1 Classical mechanics, limitations and prelude to new theories mechanics - l (M = 12)

Introductory ideas of classical mechanics – Equation of motion: Newtonian mechanics, Lagrangian mechanics, Hamiltonian mechanics, Classical mechanical Poisson bracket.
Failure of classical theories in back body radiation, specific heat of solid, photoelectric effects, and atomic spectroscopy; concept of quantization, identification of classical and quantum systems, Bohr’s correspondence principle

with examples.
de Broglie relation, concept and properties of matter wave, comparison to travelling wave, dispersion relation, uncertainty principle, Plausible arguments leading to Schrödinger equation.

Unit 2 Quantum mechanics - l (M = 22)

Postulates of Quantum mechanics; state of the system; operators, Linear operators in quantum mechanics. Eigen value equation, Hermitian operator, measurement, probability concept, and continuity equation. Stationary state, elementary applications of time independent Schrödinger equation – different potential problems: free particle, confined particle in a box, step potential barrier problem: tunneling and its applications.
Heisenberg equation of motion, constant of motion, Ehrenfest's theorem. Commutator and relationship with Poisson bracket, non-compatibility and uncertainty; Formal derivation of Heisenberg uncertainty principle: commutability and compatibility.

Quantum mechanical treatment of simple harmonic oscillator; Rigid rotator; hydrogen atom.

Approximate method: Elementary perturbation theory, Variation theorem, Simple applications.

Unit 3 Atomic structure (M = 10)

Motion of angular momentum under magnetic field. Larmor precision. Stern Gerlach experiment. Spin-orbit interaction, conservation of total angular momentum J, Zeeman effect: Normal and Anomalous.

Motion under central force: Conservation of angular momentum and its consequence. Shape of different orbits, separation of radial and angular part. Shape of orbitals

Unit 4: Dielectric properties and inter-molecular forces (M = 6)

Dielectric polarization. Mossotti-Clausius relation, polar molecule. Debye equation. Dipole moment and molecular structure. Intermolecular forces. Attraction and repulsion potentials: van der Waals forces, Keesom, Debye and

London forces, their relative contribution; Lennard-Jones potential.

References

1. Quantum Mechanics - Cohen-Tannoudji, C.; Diu, B.; Lalöe, F.,. Wiley-Interscience: Paris, 1977;
2. Quantum Mechanics Concepts and Applications, Second Edition, - Nouredine Zettili.
3. Quantum Mechanics in Chemistry - Schatz, G. C.; Ratner, M. A
4. Quantum Chemistry, 7 th Edition - Ira N. Levine.
5. Introduction to Quantum Mechanics - David J. Griffiths.
6. Quantum Chemistry: An Introduction - Walter Kauzmann.
7. Theory of electric polarization - C.J.F. Bottcher.
8. Introduction to electrodynamics - David J. Griffiths.
9. Dielectric phenomena in solids - Kwan Chi Kao.
10. Classical Mechanics - H. Goldstein.

Course learning outcomes: After the completion of the course, the students should be able to

1. Explain basic theory of classical mechanics with its failure to explain black body radiation, photoelectric effect, atomic spectra and concepts of matter waves with various arguments to reach Schrödinger equation.
2. Solve Schrodinger equation for various quantum chemical models such as, particle in a box, harmonic oscillator, rigid rotor models and H-atom,
3. Apply operator algebra to calculate eigen values and eigen functions of angular momentum
4. Apply various approximation methods to solve Schrodinger equation in presence of small perturbation and for multielectronic system.
5. Explain the idea of spin quantum number via Stern-Gerlach experiment, effect of magnetic field to atomic spectra and ideal of the shape of the orbits and orbitals.
6. explain the concept of dielectric polarization via deriving Mossotti-Clausius relation and possible intermolecular forces with their contribution.

Course No. CHEM 0891 (FM = 50; C = 4)
Organic Chemistry Lab

Course Objectives: To impart practical skill on Separation of binary organic mixtures

Separation of binary mixtures of solid-solid/liquid-solid/liquid-liquid organic compounds and identification of individual components by chemical and spectroscopic methods.

References:

1. Systematic Organic Qualitative Analysis – H. Middleton
2. Hand Book of Organic Analysis – H.T. Clarke
3. Qualitative Organic Analysis – A.I. Vogel

Course Learning Outcomes: After completion of the course, the student should be able to

1. Determine chemical composition from binary mixture of organic compounds.
2. Identify organic components by chemical and spectroscopic methods.

Course No. CHEM 0892 (FM = 50; C = 4)
Computer Application

Course Objectives: To provide basic understanding of the programming language, numerical methods, various computational techniques and to impart skills to apply them to solve problems related to chemistry.

Introduction to programming languages; basic numerical analysis: solution of nonlinear equations using Newton-Raphson method (e.g. finding the roots of a cubic equation – vander Waals equation), solution of linear systems using Gaussian elimination, interpolation, numerical integration (trapezoidal and Simpson's 1/3rd rule), numerical solution of differential equations (Euler and Runge-Kutta method). Fourier transformations and applications in spectroscopy. Use of molecular geometry optimization software (Gaussian 09); construction of z-matrix and concept of force field.

Classical Molecular Dynamics (MD) simulation and application to simple systems like Lennard-Jones fluids.

[Effort should be made to reproduce data reported in the literature using the above-mentioned numerical methods wherever possible.]

Course learning outcomes: The students will explain and acquire skills to

1. Write computer programs to solve linear systems using Gaussian elimination, interpolation, numerical integration and numerical solution of differential equations.
2. Perform Fourier transformations and its applications in spectroscopy.
3. Use quantum chemical programs to do molecular geometry optimization and frequency calculation on chemically relevant systems
4. Perform classical Molecular Dynamics (MD) simulation on biologically relevant systems.

THIRD SEMESTER

Course No. CHEM 0901 (FM = 50; C = 4)

Symmetry, Macromolecules and Magnetic Resonance

Course Objectives: The objective of this course is to provide basic knowledge of character table, material chemistry and NMR, ESR.

Unit 1 Elementary Group Theory and Application of Symmetry (M = 20)

Introduction, symmetry elements and group theory, group theory and quantum mechanics (elementary ideas), elementary ideas of representation theory, irreducible representations of point group, definitions of classes and character, statement of grand orthogonality theorem, orthogonality theorem for characters, character tables, concept of character projection operator.
Selection rules in molecular spectroscopy, electronic spectroscopy and crystal field theory. SALC – Hückel, Hybridization. Vibration of polyatomic molecules
– normal modes, their symmetry properties and IR activity.

Unit 2 Polymer Chemistry (M = 08)

Classification of polymers, kinetics of two-dimensional polymerization, condensation and addition polymerizations; initiation, propagation and termination; chain transfer, co-polymerization; molecular weight of polymers; determination of molecular weights. Thermodynamics of polymer solution: entropy, heat and free-energy of mixing.

Unit 3 Colloids and Macromolecules (M = 07)

Introduction to nanomaterial, Lyophobic and lyophilic sols, origin of charge and stability of lyophobic colloids, coagulation and Schultz-Hardy rule, zeta potential and Stern double layer (qualitative idea); Tyndall effect, electrokinetic phenomenon (qualitative idea only); Microporous materials, microgels, bioconjugate polymers, gels, ointments and creams, biodegradable polymers. Fundamentals of nano science: definition, nano versus bulk, quantum confinement: nanoscale in 1D, 2D and 3D with examples, synthesis of nano materials: top-down and bottom-up approaches, size dependent properties; nanoclusters and nanowires, semiconductor nanoparticles, applications of nano materials.

Unit 4 Spin Magnetic Resonance Spectroscopy (M = 15)

Magnetic resonance spectroscopy – introduction, basis features of spectroscopy, relaxation processes: spin-spin and spin-lattice.

NMR: chemical shift and spin-spin coupling; chemical shielding – elementary idea of diamagnetic and paramagnetic shielding.

ESR: ESR spectrometer, line width, hyper-fine splitting, ESR of triplet state, applications.

References:

1. Group theory and chemistry - D. M. Bishop.
2. Group theory and Quantum chemistry - M. Tinkham
3. Fundamentals of Polymerization - Broja Mahan Mandal
4. Principles of Polymerization - George Odian
5. Physical Chemistry - Gilbert W. Castellan
6. Physical Chemistry - K.L. Kapoor
7. Principles of Physical Chemistry - Puri Sharma Pathania
8. Physical Chemistry - P.C. Rakshit
9. Physical Chemistry - H.C. Chatterjee
10. Introduction of nanomaterials - Asim Kumar Das

Course Learning Outcomes: After completion of the course, the student should be able to

1. Elucidate point group of various geometry, construct matrix representation for point groups, character table and apply the concept to spectroscopy, crystal field theory.
2. Derive the rate expression for polymerization process, ΔS, ΔG, relative vapor pressure and explain the properties of colloidal solution, concepts of nanoscience.
3. Explain theory and instrumentation of magnetic spectroscopy and its application for chemical analysis.

Course No. CHEM 0902 (FM = 50; C = 4)
Spectroscopy, Supramolecules and Nanomaterials

Course Objectives: To impart knowledge on theory of advanced spectroscopy, basic LASER principle, spectrometry and supramolecular Chemistry

Unit 1 FT NMR, FT IR, 2D NMR, Mass spectrometry (M = 18)

Fourier transformations, time domain versus frequency domain. Principles of FT NMR, instrumentation, the rotating frame of reference, simple 1D experiments. FT IR – principles and instrumentation.

Introduction to 2D NMR: NOESY, COSY, HETCOR, HOMCOR, INADEQUATE,

INDOR, INEPT for simple compounds and problems. Applications of multinuclear NMR in inorganic compounds – Examples from ^{1}H, ^{11}B, ^{13}C, ^{19}F, ^{31}P. NMR of paramagnetic molecules – Lanthanide shift.

Mass spectrometry: Fragmentation processes and structural analysis; ESI, GC/MS, LC/MS and MS/MS techniques. Interpretation of spectroscopic (NMR, IR and mass) data, as applied to organic, inorganic and biological systems.

Unit 2 Electronic Spectroscopy (Absorption and Emission) (M = 15)

Einstein theory of Absorption and emission – A, B coefficients, Principles of LASER and characteristic features. Electric dipole transition – comparison of experimental and theoretical parameters, oscillator strength

Qualitative treatment of Born-Oppenheimer separation, Frank-Condon principle, Quantum mechanical interpretation of transition, selection rules, spin orbit coupling, vibronic coupling, characteristics of π-π^*, n-π^*, charge transfer transitions and their intensities.

Photoluminescence: fluorescence and phosphorescence, mirror-image symmetry, radiation less deactivation – internal conversion and inter system crossing. First order kinetics for excited molecule. Delayed fluorescence.

Quenching of fluorescence, Life-time variation in presence of quencher. Excimers and exciplexes. Intermolecular energy transfer. Excited state proton transfer. Modern experimental techniques in fluorescence spectroscopy.

Unit 3 Supramolecular Chemistry & Introduction to Nanomaterials (M = 09)

Introduction, Origins and Concept. Molecular recognition. Host-guest complex. supramolecular orbitals, non-covalent forces: soft interactions, Supramolecular reactivity and catalysis. Self-assembly and self-organization, Liquid crystals and supramolecular polymers, polymer-surfactant interaction. Molecular sensors and supramolecular devices.

Nanoparticles and nanomaterials, elementary idea of synthesis, nano-composites, applications (special attention in drug design). Microporous materials, microgels, bioconjugate polymers, Nanoencapsulation.

Unit 4 Mossbauer spectroscopy, PES, XPS and Applications (M = 08)

Principles of Mossbauer spectroscopy: experiments, center shift, quadrupole interaction, magnetic interaction. PES - photoexcitation and photoionization; XPS - principle and applications.

References:

1. Organic Spectroscopy - W. Kemp, ELBS
2. Introduction to Spectroscopy - Pavia, Lampman
3. Applications of Absorption Spectroscopy of Organic Compounds - Dyer
4. Spectrometric Identification of Organic Compounds - R. M. Silverstein and G. C. Bassler
5. Spectrometric method in Organic Chemistry - D.H. Williams and I. Fleming.
6. NMR Spectroscopy: Basic Principle, Concepts and Applications in Chemistry - H. Gunther, Wiley
7. Organic Structure Determination - Jeffrey H Simpson
8. NMR Spectroscopy Explained - Neil E Jacobsen
9. . Modern Molecular Photochemistry - Nicholas J. Turro
10. Principles of Fluorescence Spectroscopy, 3rd edition - Joseph R. Lakowicz.
11. Fundamentals of Photochemistry - K K. Rohotgi Mukherjee
12. Supramolecular Chemistry: Concepts and Perspectives - J. -M. Lehn

Course Learning Outcomes: After completion of the course, the student should be able to

1. Analyze the spectroscopic data, as applicable to organic, inorganic and

biological systems.
2. Analyze the possible photophysical processes for electronically excited molecules
3. Explain selection rule and their relaxation for electronic transition
4. Explore the use of supramolecular material chemistry in modern chemical society

Course No. CHEM 0903A (FM = 50; C = 4)
Advanced Organic Chemistry -I

Course Objectives: To impart advanced level knowledge on (i) stereochemical aspects of fused polycyclic systems including steroids and their application in synthesis (ii) molecular organic photochemistry including fundamental principles, primary photochemical reactions along with synthetic applications (iii) biogenesis of natural products and their role in metabolic pathways.

Unit 1: Stereochemistry of polycyclic system (M = 14)

Conformation and reactivity of fused polycyclic systems – perhydrophenanthrenes, perhydroanthracenes, steroids; Stereochemistry of reactions – nucleophilic additions to cyclic ketones, Cieplak model; directed nucleophilic additions.

Unit 2 Organic Photochemistry and Radical Reactions (M = 18)

Photochemistry: Photolysis of carbonyl compounds and nitrites: Norrish Type I and Type II processes, β-cleavage, Barton reaction. Photoreduction and Photoexcitation; Photorearrangements in cyclohexanones and cyclohexadienone systems; Photorearrangements of α-tropolone methyl ether, di-π-methane rearrangement (cyclic system) Photochemistry of organic compounds: photoisomerisation, phodimerisation, cycloadditions of benzene and its derivatives.

Radical Chemistry: Generation and detection of radicals, radical initiators, reactivity pattern of radicals, substitution, addition and cyclization reactions; Radical cations and radical anions, single electron transfer reactions.

Unit 3: Chemistry of Natural Products (Synthesis and Biosynthesis) (M = 18)

Introduction: Primary and secondary metabolites, biogenetic hypothesis, elucidation of biosynthetic pathways; Biosynthesis of terpenoids and steroids; Shikimic acid pathway: Biosynthesis of flavonoids; Biosynthesis of alkaloids; Synthesis and biosynthesis of polyketides, fatty acids and prostaglandins; Reactions and synthesis of steroids: cholesterol, bile acid, testosterone, estrone, progesterone; Structure and synthesis of porphyrins: haemoglobin, chlorophyll.

References:

1. Stereochemistry of Organic Compounds - E. L. Eliel and S. H. Wilen.
2. Stereochemistry of Carbon Compounds - E.L. Eliel and S. H. Wilen.
3. Stereochemistry of Organic Compounds: Principles and Applications - D. Nasipuri.
4. Mechanism and Theory in Organic Chemistry - Lowry and Richardson.
5. Organic Photochemistry – J. M. Coxon and B. Halton.
6. Organic Chemistry, Vol. II - I. L. Finar.

Course Learning Outcomes: After completion of the course, the student should be able to

1. Demonstrate advanced idea of stereochemistry of fused polycyclic organic compounds.
2. Implement the basics of organic photochemistry and radical chemistry.
3. Interpret structures, laboratory and biosynthetic pathways for the generation of several primary, secondary metabolites and complex natural products.

Course No. CHEM 0903B (FM = 50; C = 4)

Advanced Inorganic Chemistry -I

Course Objectives: To provide the knowledge on applications of group theory, various aspects of magnetochemistry, solid-state chemistry

Unit 1 Chemical Application of Group Theory (M = 17)

Importance of group theory in inorganic chemistry, splitting of orbital and free ion terms in crystal fields, quantitative relationship between Oh & Td splittings, construction of energy level in infinitely strong crystal field, the effect of distortion on d-energy levels, vibronic coupling and vibronic polarization, utilization of symmetry and group theory in constructing the MO diagrams of polyatomic molecules, coordination complexes including metallocene complexes. Symmetry of normal vibration, normal mode analysis, selection rules for IR and Raman transitions.

Unit 2 Magnetochemistry (M = 18)

Definition of magnetic properties, types of magnetic bodies, Curie equation, Curie's law and Curie-Weiss law. Anisotropy in magnetic susceptibility, diamagnetism in atoms and polyatomic system, Pascal's constants, two sources of paramagnetism, spin and orbital effects, spin-orbit coupling, Lande interval rule, energies of *J* levels, first order and second order Zeeman effects, temperature independent paramagnetism, simplification and application of van Vleck susceptibility equation, quenching of orbital moment, magnetic properties of transition metal complexes, low spin, high-spin crossover, magnetic behavior of lanthanides and actinides, magnetic exchange interactions. Experimental arrangements for determination of magnetic susceptibility: SQUID. Preliminary idea about single molecular magnets.

Unit 3 Solid state chemistry and X-ray crystallography (M = 15)

Bonding in metal crystals: free electron theory, electrical conductivity, band theory, band gap, metal and semi-conductors – intrinsic and extrinsic semiconductors; semiconductor/metal transition, p-n junctions, superconductivity, Bardeen, Cooper and Schriefer (BCS) theory. Dia-, para- and ferromagnetism. Defects in solids.

The geometry of crystalline state; Nature and generation of X-rays, Production of monochromatic X-rays, Scattering of X-rays, Diffraction of X-rays by crystals, Bragg's law, 1, 2 and 3 dimensional Laue equations, atomic scattering factor, structure factor, systematic absences, Determination of space groups and crystal structures.

References:

1. Chemical Applications of Group Theory - F. A. Cotton.
2. Magnetochemistry - A. Earnshaw.

3. Elements of Magnetochemistry - R. L. Dutta, A. Shyamal.
4. An Introduction to X-Ray Crystallography - M. M. Woolfson.
5. X-Ray Diffraction Methods - E. W. Nuffield.
6. X-ray Crystallography - M. J. Buerger.
7. Solid State Chemistry - D. K. Chakrabarty.
8. Crystallography Applied to Solid State Physics - A. R. Verma & O. N. Srivastava.
9. Structure of Metals - Charles Barret & T. B. Masalski.
10. Introduction to materials Science for Engineers - J. F. Shakelford & M.K. Muralidharan.
11. Superconductivity - R. G. Sharma.
12. Physical Chemistry - I. R. Levine.
13. Theoretical Chemistry - S. Glasstone

Course Learning Outcomes: On completion of the course, the students should be able to

1. Apply group theory to understand the vibrational spectroscopy of different complexes and CFT of coordination complexes.
2. Analyze the magnetic properties of different mononuclear and polynuclear metal complexes.
3. Measure the magnetic properties using SQUID.
4. Describe the origin of the conductivity in metallic conductors, semiconductors and superconductors.
5. Explain the molecular origin of dia-, para- and ferromagnetisms.
6. Quantify the extent of defects in solids.
7. Gain a comprehensive knowledge on the interaction between X-rays and crystalline solids and determine the space groups of crystals.

Course No. CHEM 0903C (FM = 50; C = 4)
Advanced Physical Chemistry -I

Course Objectives: To impart knowledge of various statistics, dielectric behavior, solvent effect on spectra, structures of solids and different rate processes.

Unit 1 Statistical mechanics- II (M = 15)

Concept of the macroscopic and the microscopic states, Statistical conditions for thermal, mechanical and chemical equilibrium; and connection between total micro-states and thermodynamics key quantities.

Concept of ensemble and ergodic hypothesis, phase space; microcanonical ensemble, counting micro-states, Gibbs paradox, correct enumeration of the microstates, Sackur-Tetrode equation;

Canonical ensemble distribution, probability distribution function, its relation with different thermodynamic state functions; application to a system of harmonic oscillators; the statistics of paramagnetism, energy fluctuations in the canonical ensemble, equipartition and the virial theorem. chemical potential and chemical equilibrium – Saha ionization formula;

Grand canonical ensemble – Density and energy fluctuations in the grand canonical ensemble: correspondence with other ensembles; phase equilibrium.

Nature of quantum particles; Bose-Einstein and Fermi-Dirac distributions; black body radiation and photon gas, Bose-Einstein condensation; Thermodynamic behavior of an ideal Fermi gas; the electron gas in metals.

Unit 2 Dielectric behaviour and solvent effect (M = 10)

Limitation of Mossotti-Clausius, Debye equation, deviation from Debye's theory; Onsager reaction field; dielectric relaxation, frequency dependent dielectric property, relaxation time, Debye semicircle; Solvent effect on the emission and absorption spectra - non- specific and specific interactions (H-bonding and charge transfer). Lippert equation; time resolved spectroscopy and the solvent relaxation.

Unit 3 Solid state chemistry and X-ray crystallography (M = 15)

Bonding in metal crystals: free electron theory, electrical conductivity, band theory, band gap, metal and semi-conductors – intrinsic and extrinsic semiconductors; semiconductor/metal transition, p-n junctions, superconductivity, Bardeen, Cooper and Schriefer (BCS) theory. Dia-, para- and ferromagnetism. Defects in solids.

The geometry of crystalline state; Nature and generation of X-rays, Production of monochromatic X-rays, Scattering of X-rays, Diffraction of X-rays by crystals, Bragg's law, 1, 2 and 3 dimensional Laue equations, atomic scattering.factor, structure factor, systematic absences, Determination of space groups and crystal structures.

Unit 4 Kinetics - II (M = 10)

(a) Rate constant expression for chemical reaction based on Eyring equation with one example.
(b) Physical rate processes – viscosity and diffusion.
(c) Non- equilibrium formulation: Passage to statistical approach – energy redistribution in activated complex, Lindemann collision, Hinshelwood suggestion, Rice-Ramsperger-Kassel (RRK) theory.
(d) Reaction in solution. Diffusion-controlled reactions.

References

1. Statistical Mechanics – R. K. Pathria.
2. Introduction to Statistical Physics - Kerson Huang.
3. Fundamentals of statistical and thermal physics – F. Rief.
4. Statistical Mechanics - Donald A. McQuarrie.
5. An Introduction to Statistical Thermodynamics - Terrell L. Hill
6. Statistical Mechanics and Thermodynamics - Claude Garrod.
7. Heat and Thermodynamics – M. W. Zamansky, and R. H. Dittman.
8. Theory of electric polarization, - C. J. F. Bottcher.
9. Introduction to electrodynamics - David J. Griffiths
10. Dielectric phenomena in solids - Kwan Chi Kao.
11. An Introduction to X-Ray Crystallography - M. M. Woolfson.
12. X-Ray Diffraction Methods - E. W. Nuffield.
13. X-ray Crystallography - M. J. Buerger.
14. Solid State Chemistry - D. K. Chakrabarty.
15. Crystallography Applied to Solid State Physics - A. R. Verma and O. N. Srivastava.
16. Structure of Metals - Charles Barret and T. B. Masalski.
17. Introduction to materials Science for Engineers - J. F. Shakelford & M. K. Muralidharan.
18. Superconductivity by R. G. Sharma.
19. Physical Chemistry - I. R. Levine.
20. Theoretical Chemistry - S. Glasstone.
21. Chemical Kinetics - Keith J. Laidler.

22. The Theory of Rate Processes - Samuel Glasstone , Keith J. Laidler , Henry Eyring.
23. Dielectric Properties and Molecular Behaviour - Nora Hill
24. Principles of Fluorescence Spectroscopy - Joseph R. Lakowicz.

Course learning outcomes: After the completion of the course, the students should be able to

1. Describe the various ensembles equipartition theorem and its validity, Saha ionization formula, correlate Bose-Einstein and Fermi-Dirac statistics.
2. Express the limitation of Mossotti-Clausius equation, role of solvent to absorption- emission spectra and explain the time resolved emission spectra due to solvent relaxation.
3. Explain the molecular origin of dia-, para- and ferromagnetisms.
4. Quantify the extent of defects in solids.
5. Gain a comprehensive knowledge on the interaction between X-rays and crystalline solids and determine the space groups of crystals.
6. Apply Eyring equation, explain the behavior of diffusion-controlled reactions and Lindemann collision, RRK theory

Course No. CHEM 0991A (FM = 50; C = 4)

Advanced Organic Chemistry Lab

Course Objectives: To impart hands on training on multistep synthesis of organic compounds and their characterization

Multistep synthesis of organic compounds using typical organic reactions, purification and characterization of the product [by re-crystallization, TLC, PC, determination of R_f value as required, m.p/b.p.]. Characterization of organic compounds by spectroscopic means.
Extraction and Purification of Natural Products and Biomolecules.

References:

1. Systematic Organic Qualitative Analysis – H. Middleton
2. Hand Book of Organic Analysis – H.T. Clarke
3. Qualitative Organic Analysis – A.I. Vogel

Course Learning Outcomes: After completion of the course, the student should be able to

1. Deal with various synthetic problems
2. Handle sophisticated chemicals for synthetic application
3. Improve their analytical skills for separation and characterization.

Course No. CHEM 0991B (FM = 50; C=4)

Advanced Inorganic Chemistry Lab

Course Objectives: The course aims to provide practical knowledge on analysis of ores, minerals and alloys, synthesis and characterization of some interesting transition metal complexes.

1. Quantitative analysis of complex inorganic materials *viz.* ores, minerals and alloys etc. by conventional method. (any one)
2. Synthesis and characterization of Inorganic Compound
3. Preparation of transition metal complexes and their characterization

Course Learning Outcomes: On completion of the course, the students should be able to

1. Analyze the components of alloys, ores etc.
2. Able to handle the apparatus in synthetic lab
3. Able to interpret the characterization data

Course No. CHEM 0991C (FM = 50; C = 4)

Advanced Physical Chemistry Lab

Course Objectives: To provide hand-on experiences of techniques for verifying physical and chemical properties.

1. Tensiometry

2. Autocatalysis

3. Fluorescence quenching

4. Excited State Proton Transfer

5. Resonance Energy Transfer

6. Kinetic Salt effect

7. Onsager Theory (updated and modified version) – Conductance measurement

8. Solubility Product – Conductance measurement

9. Ternary Phase diagram

10. Clock reaction

Course learning outcomes: The students will acquire skills to

1. Evaluate rate constant, rate constant at zero ionic strength and Debye Hückel constant by spectrophotometry instrument for ionic reaction.
2. Elucidate individual order of the reactants for redox reaction by clock method.
3. Plot ternary phase diagram on two dimensions for water, chloroform, acetic acid system.

Course No. CHEM 0992 (FM = 50; C = 4)

Research Based Lab

Course Objectives: The course aims to provide advance practical/hands-on skills on the active research fields in departmental research laboratories to enhance their employability scope in academia and industry. Some of the active research areas are given below.

1. Synthetic organic chemistry
2. Synthetic inorganic and material chemistry.
3. Energy storage device
4. Polymer Chemistry
5. Computational Chemistry
6. Theoretical Chemistry
7. Spectroscopy
8. Environmental Chemistry

Course Learning Outcomes: On completion of the course, the students should be able to

1. Explore current research problems
2. Prepare themselves to handle research projects

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FOURTH SEMESTER

Course No. CHEM 1001A (FM = 50; C = 4)

Advanced Organic Chemistry -II

Course Objectives: This course aims to foster an understanding of (i) the key aspects of coordination compounds of transition metals along with a detailed knowledge of catalytic and industrial uses of organometallic compounds (ii) the importance of asymmetric synthesis, the concept, the biological relevance and a critical knowledge about the synthetic strategies available to us (iii) advanced level target-oriented synthesis of biologically relevant molecules employing various modern reagents.

Unit 1: Organotransition Metal Chemistry: Applications to Organic Synthesis (M = 17)

Electron counting, bonding, organometallic reaction mechanism; Homogeneous hydrogenation; Organometallics as electrophiles; Synthetic applications of transition metal alkene complexes: Wacker oxidation. Synthetic applications of complexes containing metal – carbon σ bonds: Heck and related reactions, carbonylation reactions; Synthetic applications of transition metal carbene complexes: Fischer carbene, Schrock carbene, metathesis processes, Tebbe's reagent, Zieglar – Natta reaction; Synthetic applications of transition metal alkyne complexes: Pauson – Khand reaction, cyclooligomerisation; Applications of transition metal complexes in the synthesis of: cyclic enediynes, estrone by Volhardt, clavicipitic acid by Hegedus.

Unit 2: Asymmetric Synthesis (M = 16)

Principles; Addition to carbonyl compounds: use of chiral substrate, chiral reagent, chiral catalyst; Stereoselective reactions of carbonyl compounds: enolate formation, alkylation, asymmetric aldol reactions; Stereoselective reactions of alkenes: Diels-Alder reaction, sigmatropic rearrangement, stereoseletive hydrogenation, epoxidation, hydroxylation, aminohydroxylation, cyclopropanation; Kinetic resolution; Asymmetric synthesis of menthol (Takasago), crixivan (Merck)

Unit 3: Synthesis of complex and biologically important molecules Applying Modern reagents and methodologies (M = 17)

A. **Organic synthesis**: (i) Target-oriented synthesis – natural products, designed molecules (ii) Method-oriented synthesis – reagents, catalysts, synthetic strategies and tactics. Retrosynthetic analysis: Selected total synthesis of natural products like Taxol, Tetracycline antibiotics etc.

B. **Synthetic methodology and strategy of few compounds**: (i) cationic cyclisations: progesterone (Johnson) (ii) radical cyclisations: synthesis of hirsutene (Curran) (iii) pericyclic reactions: endiandric acids (Nicolaou); (iv) Photochemical reactions: strained compounds (isocomene by Pirrung) (v)aldol reactions: Prelog-Djerassi lactone; (vi) carbene reactions: making cyclopropanes (vii) biomimetic strategy: carpanone (Chapman) (viii) solid-supported reagents, solid phase synthesis: plicamine (Ley) (ix) combinatorial synthesis etc.

References:

1. Organic Chemistry, Vol. II - I. L. Finar, ELBS
2. Organotransition Metal Chemistry: Applications to Organic Synthesis - S. G. Davis, Pergamon
3. Transition Metals in the Synthesis of Complex Organic Molecules - L. S. Hegedus, USB
4. The Organometallic Chemistry of the Transition Metals: R. H. Crabtree.
5. Principles And Applications Of Asymmetric Synthesis – G.-Q. Lin; Y.-M. Li; A. S. C. Chan, A John Wiley & Sons, Inc.
6. Organic Chemistry - J. Clayden, N. Greeves and S. Warren, Oxford University Press, 2nd Ed, 2012.
7. Asymmetric synthesis: J.D. Morrison, Vol 1-5, Academic press, 1983.
8. Stereochemistry of Carbon Compounds - E.L. Eliel and S.H.Wilen, McGraw Hill Education, 2001.
9. Comprehensive asymmetric catalysis - Jacobson, E. N.; Pfaltz, A.; Yamamoto, H. Eds.), Springer 2000.
10. Asymmetric catalysis in organic synthesis: R. Noyori, Wiley-NY 1994.
11. Catalytic asymmetric synthesis: I. Ojima, VCH-NY, Pergamon, 1998.
12. Methods for the asymmetric synthesis of complex organic molecules: Daniel, J. O’Leary, Lecture Notes 2001.
13. Principles of Asymmetric Synthesis (Tetrahedron series in Organic Chemistry), R. E. Gawley, J Aube, Pergman, 1996.
14. Classics in Total Synthesis: Targets, Strategies, Methods: K. C. Nicolaou, E. J. Sorensen, Wiley, 1996.

15.Classics in Total Synthesis II - K.C. Nicolaou and S.A. Snyder Wiley-VCH.

Course Learning Outcomes: After completion of the course, the student should be able to

1. Implement the idea of Organotransition Metal Chemistry for synthesis of Organic compounds.
2. Enhance broad understanding of stereochemistry, biological relevance of isomers, resolution, importance of asymmetric synthesis using chiral auxiliary, asymmetric catalysis, chiral ligand designing etc. They will reach upto the frontier knowledge about the importance of synthesizing enantiomerically pure organic compounds and strategies available for this purpose.
3. Explore various synthetic methodologies and strategies for the preparation of complex and biologically important molecules.

Course No. CHEM 1001B (FM = 50; C = 4)

Advanced Inorganic Chemistry -II

Course Objectives: To impart the knowledge of spectroscopic analysis for inorganic systems, advance functional materials and nanomaterials

Unit 1 Spectroscopy - Applications to Inorganic Systems (M = 25) Electronic spectroscopy: Orgel diagrams, correlation between weak field and strong field terms. Tanabe-Sugano diagram, bonding parameters and structural evidences from electronicspectra of d-metal complexes, f-f transition, lanthanide and actinide spectra. Applications of IR, Raman, ESR and Mossbauer spectroscopy to inorganic and bioinorganic systems, NMR spectra: ^{11}B, ^{13}C, ^{19}F, ^{27}Al, ^{31}P NMR spectroscopy with typical examples, ^{1}HNMR spectra of coordination compounds of paramagnetic metal ions, dipolar and contact shifts, magnetic susceptibility and resonance shift. NQR spectroscopy: Principle, nuclear quadruple coupling constants, structural information from NQR spectra. Applications of CD and MCD; stereoselective and stereospecific effects.

Unit 2 Advanced Functional Inorganic Materials (12)

Metal complexes: with salan, salen and salophen types of ligands: synthesis, properties and applications. Supramolecular chemistry: Introduction to Metal Organic Frameworks (MOFs), design of simple and functional MOFs by postsynthetic modification, tuning of their structure, properties and various recent applications.

Unit 3 Advanced Inorganic Nanomaterials (13)

Introduction to nanomaterials, Surface area and quantum effects in nanomaterials. Conventional types of nanomaterials: carbon based, metal based, dendrimer based, and composite based. Nanomaterials synthesis and processing: Top-Down and bottom-up approach. Chemical Analysis of nanomaterials: Energy dispersive X-ray spectroscopy (EDS/EDX); Xray photoelectron spectroscopy (XPS), X-ray diffraction. Atomic absorption spectroscopy (AAS); inductively coupled plasma-atomic emission spectroscopy (ICP-AES), temperature programmed desorption (TPD); Thermogravimetric analysis (TGA) Basic concepts in surface imaging; secondary electron microscopy (SEM); scanning tunnelling microscopy (STM); transmission electron microscopy (TEM), atomic force microscopy (AFM) Optical property study: photoluminescence, FTIR, Raman spectroscopy.

Application of inorganic nanomaterials in catalysis, environmental remediation, sensing, biotechnology etc.

References

1. Inorganic Spectroscopic Methods - Alan K Brisdon.
2. Physical Methods for Chemists - R. S. Drago.
3. Fundamentals of Molecular spectroscopy - N. Banwell, E. M. McCash.
4. Inorganic Nanomaterials: Synthesis Characterization and Applications – M. Zhang.
5. Inorganic Nanoparticles: Synthesis, Applications, and Perspectives - Altavilla, E. Ciliberto.
6. The Chemistry of Nanomaterials: Synthesis, Properties and Applications - N. Rao, A. Muller, A. K. Cheetham.

Course learning outcome: After the completion of the course, the students should be able to

1. Rationalize the spectral properties of inorganic materials with appropriate theory
2. Explain the structure-property relationship of inorganic or bioinorganic systems by spectroscopic methods
3. Design the novel functional materials and analyse the characterization data
4. Explain the principle of nanosizing, design the nanomaterials and analyse the characterization data

Course No. CHEM 1001C (FM = 50; C = 4)
Advanced Physical Chemistry -II

Course Objectives: To acquire knowledge of many electron system, irreversible thermodynamics, trajectory for collision and electrode-solution interface.

Unit l Quantum Mechanics - II (M = 10)

Vector space, matrix representation of operators, Hermitian operators and matrices, Virial theorem, parity, time reversal symmetry; angular momentum operator – commutation relation, set-up and set-down operators, angular momentum operators in polar coordinates, angular momentum eigenfunctions: solutions from corresponding eigenvalue equation.
Many electron Hamiltonian, its communication with composite L^2 and Lz; spin operator and Pauli spin matrices; many electron atom and construction of wavefunction representing spectroscopic state; projection operators and their properties – projection operator technique and angular momentum.

Unit 2 Non-equilibrium phenomena (M = 15)

(a) Einstein's theory of Brownian motion; Diffusion and mobility, Perrin experiment, Determination of Avogadro number, Deduction of equation of motion for Brownian particles - Langevin's description, System bath equilibrium - fluctuation dissipation relation, General expression for mean square displacement, Probabilistic description of Brownian motion - Fokker-Planck equation; solution for free particles.

(b) Binomial, Poisson, and Gaussian distributions - generating functions, moment generating function, Characteristic Function, Cumulant Generating Function, The Central Limit Theorem.

(c) Classical Linear Response Theory, Properties of the Response Function, Causality, stationarity, impulse response, The Susceptibility, Kramers–Krönig relations, Application to a Driven Harmonic Oscillator; Quantum Linear Response Functions.; The Response Function and Energy Absorption, Relaxation of a Prepared State

Unit 3 Molecular Reaction Dynamics (M = 10)

Reaction dynamics: Introduction, molecular dynamics – intermolecular collision and its consequence; role of intermolecular potential, reaction cross-section, energy threshold, reaction probability; angular distribution in relative collision; scattering in velocity space; electronic energy transfer; experimental methods in connection with molecular dynamics; chemiluminescence; chemical laser; crossed molecular beam; photofragmentation spectroscopy.

Unit 4 Advanced Electrochemistry (M = 15)

Limitation of Debye-Hückel limiting law and its extension; Pitzer ion- interaction approach. Debye-Hückel-Onsagar (DHO) theory of electrical conduction of electrolytes, electrophoretic and relaxation effects, Wien effect, Debye-Falkenhagen effect, application of DHO theory. Limitation of DHO equation and Shedlovsky approach.

Double layer studies: nature of the double layer across electrode-solution interface, polarizable and non-polarizable electrodes, electrocapilarity (EC) – nature of EC curves, its thermodynamics, Lipmann equation, Helmholtz, Guoy- Chapman and Stern double layer models. Electron transfer reactions; fuel cells.

References:

1. Quantum Mechanics Concepts and Applications, Second Edition, - Nouredine Zettili.
2. Quantum Mechanics in Chemistry – G. C. Schatz and M. A. Ratner.
3. Quantum Chemistry, 7 th Edition, - Ira N. Levine.
4. Introduction to quantum mechanics - David J. Griffiths.
5. R. K. Pathria - Statistical Mechanics.
6. Einstein A 1956 Investigations on the theory of Brownian movement edited by R. Furth (Dover, NewYork) [Papers I and Chandrasekhar S 1943 Stochastic problems in Physics and Astronomy, Rev. Mod. Phys.15 1
7. Chemical Dynamics in Condensed Phases - Nitzan, A.
8. Gardiner, Handbook for stochastic methods: for physics, chemistry and natural sciences
9. Modern Electrochemistry 1: Ionics - J.O.M. Bockris; A. K. N. Reddy (Springer)
10. Modern Electrochemistry 2A: Fundamentals of Electrodics - J.O.M. Bockris; A. K. N. Reddy (Springer)
11. Modern Electrochemistry 2B: Electrodics in Chemistry, Engineering, Biology, and Environmental Sciences - J.O.M. Bockris; A. K. N. Reddy.

12. An Introduction to Electrochemistry - S. Glasstone.
13. Textbook of Physical Chemistry - S. Glasstone.

Course learning outcomes: After the completion of the course, the students should be able to

1. Represent quantum mechanical operators in the matrix form
2. Solve eigen value-eigen functions using matrix algebra
3. Explain Brownian motion in velocity space, properties of thermodynamic fluctuations, laws of irreversible thermodynamics and their application.
4. Express for energy dependent collision cross section, classical trajectory for bimolecular collision with angular distribution of products and concept of opacity function, chemical laser.
5. Describe quantitatively how the activity coefficients of electrolyte solutions upto saturation vary with concentration.
6. Explain the theory of conduction of electricity in electrolyte solutions.
7. Explain the behaviour of electrical double layers

Course No. CHEM 1002A (FM = 50; C = 4)
Advanced Organic Chemistry -III

Course Objectives: This course aims to (i) provide critical knowledge about target-oriented synthesis of complex heterocyclic scaffold and medicinally important molecules (ii) deal with the essentials of chemistry and biology of important class of biomolecules: nucleic acids, proteins and enzymes enabling the students to learn more advanced topics of biology including structural biology, biotechnology, genomics and proteomics etc.

Unit 1: Advanced Heterocyclic Chemistry (Two and more heteroatom) (M = 17)

Synthesis and reactivity of 5,6-membered rings containing two heteroatoms, pyrimidines and purines. Introduction to chemistry of azepins, oxepins, thiepins and their analogues; phosphorous and selenium containing heterocycles with the use of modern reagents. ANRORC and Vicarious nucleophilic substitutions in heterocycles.

Unit 2: The molecules of life (M = 16)

Introduction: The molecules of life – nucleic acids, proteins and enzymes, carbohydrates, lipids. Mechanism in biological chemistry: (i) Mechanism of enzyme action, examples of enzyme mechanisms for chymotrypsin, ribonuclease, lysozyme and carboxypeptidase A (ii) Enzyme catalysed reactions – examples of nucleophilic displacement on a phosphorus atom, coupling of ATP cleavage to endergonic processes, proton transfer reactions to and from carbon (iii) Mechanism of reactions catalysed by cofactors including coenzyme A, NAD^+, NADH, FAD and thiamine pyrophosphate; Chemical synthesis of peptides and proteins; Use of enzymes in organic synthesis; Structural analysis of proteins; Protein folding; Biotechnological applications of enzymes: Enzyme purification, immobilization of enzymes, enzyme therapy, enzyme and recombinant DNA technology.

Unit 3: Chemistry of Medicinally Important Molecules (M = 17)

Bacterial and animal cells, antibacterial agents – mechanism with reference to β-lactam antibiotics; General method of synthesis of β-lactam ring: synthesis ofpenicillin, 6-APA, cephalosporin, 7-ACA; Morin – Jackson rearrangement; Structure-activity relationship of penicillin. New generation antibiotics / antibacterial agents: Synthesis and mechanism of action of (i) fluoroquinolones – norfloxacin, ciprofloxacin, levofloxacin (ii) anti AIDS drugs – AZT, lamivadine (iii) antihypertensive agent – captopril (iv) calcium channel blocker – amlodipine (v) gastric secretion inhibitor – omeprazole (vi) drug for impotency – sildenafil etc.

References:

1. Heterocycles in Organic Synthesis - A.I. Meyers, Wiley
2. Heterocyclic Chemistry - J.A. Joule and K. Mills, Blackwell
3. Heterocyclic Chemistry - T.L. Gilchrist, Wiley
4. Organic Chemistry, Vol. I and II - I. L. Finar, ELBS
5. Lehninger Principles of Biochemistry: David L. Nelson, Michael M. Cox.
6. Fundamentals of Biochemistry: Life at the Molecular Level: Donald Voet, Judith G. Voet, Charlotte W. Pratt.
7. Burger's Medicinal Chemistry, Drug Discovery and Developments (Vol 1-8) by Burger and Burger
8. The Organic Chemistry of Drug Design and Drug Action - R. B. Silverman
9. Top Drugs: Their History, Pharmacology and Synthesis - Ji Jack Li
10. Beta lactams (Vol I and II) - A.K. Bose and M. S. Manhas
11. Medicinal Chemistry - G. L. Patrick

Course Learning Outcomes: After completion of the course, the student should be able to

1. Explore advanced Heterocyclic Chemistry of sulphur, selenium, oxygen, nitrogen containing organic compounds including puring, pyrimidines.
2. Develop the knowledge of the molecules of life – such as nucleic acids, proteins and enzymes, carbohydrates, lipids and their Mechanism in biological chemistry.
3. Use sophisticated methods of preparation to prepare modern medicinally important molecules

Course No. CHEM 1002B (FM = 50; C = 4)
Advanced Inorganic Chemistry -III

Course Objectives: To impart the knowledge of inorganic reaction mechanisms, bioinorganic chemistry and advance materials for energy storage

Unit 1 Inorganic Reaction Mechanism (M = 25)

Mechanism of substitution reactions: Solvent exchange, aquation, anation, base hydrolysis, acid catalysed aquation, pseudo-substitution. Four board classes of mechanism of substitution – 'D', 'A', 'Ia' and 'Id' Mechanism of isomerisation reaction–linkage isomerism, cis-trans isomerism, intramolecular and intermolecular racemisation, Ray– Dutta and Bailar twist mechanisms. Mechanism of electron transfer reactions: General characteristics and classification of redox reactions, selfexchange reactions. Outer sphere and inner sphere reactions, applications of Marcus expression (simple form), redox catalysed substitution reactions.

Inorganic Photochemistry: Excitation modes in transition metal complexes, fate of photo excited species; photochemical processes: Photosubstitution and photoelectron transfer reactions in Co, Cr and Rh-complexes.

UNIT 2 Advance materials for energy storage (M=10)

Classifications of energy storage devices-batteries and supercapacitors; Energy storage mechanisms; Materials design for energy storage; Cyclic voltammetric and electrochemical impedance spectroscopic characterizations for energy materials; Classification of batteries-primary and secondary; Mechanisms of lead-acid and lithium-ion batteries; Classifications of supercapacitors; Electrical double layer capacitors; pseudocapacitors; hybrid capacitors; Applications of energy storage devices

Unit 3 Bioinorganic Chemistry (M = 15)

Uniqueness of metal ion as bioelements. Interaction of metal ions with biomolecules, Metalloproteins and metalloenzymes Oxygen uptake proteins:- hemoglobin and myoglobin; Electron transport proteins: – cytochromes (specially cytochrome C), ferridoxins; metalloenzymes: – catalase, peroxidase, superoxide dismutase (SOD), cytochrome C oxidase, carbonic anhydrase, carboxypeptidase; respiratory electron transport chain and photosynthetic electron transport chain, Toxic metal ions and their effects, chelation therapy, Pt and Au complexes as drugs, metal dependent diseases.

References

1. Electrochemical Supercapacitors: Scientific Fundamentals and Technological Applications - B. E. Conway
2. Lithium-Ion Batteries: Science and Technologies - M. Yoshio, R. J. Brodd and A. Kozawa
3. Lead-Acid Batteries: Science and Technology - D. Pavlov
4. Bioinorganic Chemistry - Asim K Das
5. Selected Topics in Inorganic Chemistry - W. U. Malik, G. D. Tuli, R. D. Madan.

Course learning outcomes: After the completion of the course, the students should be able to

1. Explain the mechanistic pathway of inorganic reactions for coordination compounds
2. Explain functioning of important enzymes and proteins in our body and have ideas of metal-based drugs and their side effects.
3. Have ideas of metal induces pollution to environment & living system and some possible remedy.
4. Explain the fundamental concepts of batteries and supercapacitors
5. Design the optimized hybrid device based on the targeted application

Course No. CHEM 1002C (FM = 50; C = 4)
Advanced Physical Chemistry -III

Course Objectives: To impart knowledge about advance quantum chemistry, selection rule, symmetry operators in vector space and utilization of the great orthogonality theorem.

Unit 1 Quantum mechanics - III (M = 15)

Perturbation theory (PT) – Rayleigh-Schrödinger PT for non-degenerate states theorem, some simple applications: expression for polarizability, ground state of helium atom; degenerate state PT – Stark effect, lifting of degeneracy by application of a magnetic field (e.g., the ^{1}P1 state of helium atom) variation method – Euler variation, principle and Rayleigh-Ritz variation theorem, applications. Hückel Molecular Orbital theory for π-conjugated system.
Quantum chemistry: Born-Oppenheimer approximation, theories of valence, the MO and VB methods for H2 molecule – their relative merits, dissociation curve, excited state, configuration interaction.
Many electron systems – its characteristics, independent particle model (IPM), Hartree and Hartree-Fock methods for closed shell (elementary ideas). Basics of Density Functional Theory.

Unit 2 Quantum mechanics and spectroscopy (M = 20)

Time dependent perturbation theory – semiclassical treatment of interaction of matter with radiation, first and second order effects, Fermi golden rule, selection rule, selection rule for vibrational spectra, anharmonicity correction by perturbation – appearance of overtones; selection rule for rotational spectra, nucleur spin and rotational energy levels, stark effect revisited.
Raman scattering: selection rule for rotational and vibrational raman spectroscopy.
Quantum mechanical theory of magnetic resonance; Bloch equations and their solutions; theories of shielding – diamagnetic and paramagnetic shielding.

Unit 3 Advanced Group theory (M = 15)

Representation of symmetry operator – transformation of basis vector, general vector and functions under symmetry operations; symmetry transformation of operators and operator equation; invariance of the Hamiltonian under symmetry operation; vector space and representation theory, reducible and irreducible representations, concepts of classes and character; Wave functions as the basis of irreducible representations.

Great orthogonality and related theorems, construction of character table, reduction formula and projection operators, direct product representation, theorem on vanishing matrix elements; applications of the projection operator technique and the direct product representation.

References

1. Quantum Mechanics Concepts and Applications, Second Edition, - Nouredine Zettili.
2. Quantum Mechanics in Chemistry - G. C. Schatz and M. A. Ratner.
3. Quantum Chemistry, 7 th Edition, - Ira N. Levine.
4. Introduction to quantum mechanics - David J. Griffiths.
5. Molecular Spectroscopy - Ira N. Levine.
6. Molecular Quantum Mechanics - P. W. Atkins, R. S. Friedman.
7. Chemical Applications of Group Theory - F. A. Cotton.
8. Group Theory and Chemistry - D. M. Bishop.

Course learning outcomes: After the completion of the course, the students should be able to

1. Explain the concept of Perturbation theory for degenerate and nondegenerate states,
2. Apply the approximation methods to solve the Schrodinger equation of many electron systems and their application for to describe the concept of bonding.
3. Describe selection rule for rotational, vibrational and vibrational Raman spectroscopy, concept of Bloch equations and their solutions.
4. Express matrix representation of operators using vector space, reducible, irreducible and direct product representation.
5. Apply projection operator technique in molecular system.

Course No. CHEM 1003 (FM = 50; C = 4)
Seminar/Review and Grand Viva

Course Objective: To provide training on the scientific presentation and group discussion skills which will help them to prepare for job interviews in academia and industries.

1. Poster presentation/Seminar/Review (M = 30)
2. Grand viva (M = 20)

Course learning outcomes: On completion of the course, the students should be able to

1. Present scientific topics in an organized manner
2. face the job interviews in a confident manner.

Course No. CHEM 1091 & CHEM 1092 (FM = 50 + 50)
Project dissertation, presentation, defense and proposal

Course Objective: To provide training for literature survey, experimental and theoretical research work, instrumental techniques and their operational procedure useful for their employability in industry and academia and also to orient them for future PhD programs.

Course No. CHEM 1091 (FM=50)
Project dissertation

The students will be carrying out a project work of 4 months duration in any of the research laboratory in the Department of chemistry according to their interest and availability of the position. This dissertation has to be submitted in the form of a thesis. The M. Sc. thesis will have two chapters. The chapter 1 will contain detail literature survey on the project topic and chapter 2 will contain the origin of the project work, methodology, results and discussion and conclusions. The training and the M. Sc. thesis of these students will then be evaluated.

Course No. CHEM 1092 (FM=50)

Project presentation, defense, proposal

1. Project presentation and defense (M = 40)
2. Short project proposal (M =10)

Course learning outcomes: On completion of the course, the students should be able to

1. Explore new areas of research in both chemistry and allied fields of science and technology
2. Perform literature survey for the research topic of his/her area of expertise.
3. Rationalize the research gap for new innovation.
4. Comprehend expertise for writing the research reports.
5. Expose safe laboratory practices by handling high end equipment and chemical reagents.