

Gauhati University

B.Sc. with Chemistry

&

Chemistry as Generic

Elective

Choice Based Credit System (CBCS)

Course effective from academic year 2019-20

This is approved in the Academic Council held on 08/11/2019



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Gauhati University

Guwahati::Assam

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Preamble

The choice based credit system is naturally the next logical step in a credit based semester system. This makes the system the more learner-centric. A CBCS offers the student a diversity of courses to choose from and the autonomy to decide on the place, pace and the time of learning.

The Gauhati University has decided to introduce the CBCS system at the under graduate level from the session 2019-20. The CBCS syllabus for the B.Sc. (Regular) is prepared in the model of syllabus prepared by the UGC.

Course Structure, B.Sc. with Chemistry

Course	*Credits	
	Theory+ Practical	Theory + Tutorial
I. Core Course Theory (12 Papers) 04 Courses from each of the 03 disciplines of choice Core Course Practical/ Tutorial* (12 Papers) 04 Courses from each of the 03 disciplines of choice	$12 \times 4 = 48$ $12 \times 2 = 24$	$14 \times 5 = 60$ $12 \times 1 = 12$
II. Elective Course (6 Papers) Two papers from each discipline of choice including paper of interdisciplinary nature.) Elective Course Practical / Tutorials* (6 Practical / Tutorials*) Two papers from each discipline of choice including paper of interdisciplinary nature.)	$6 \times 4 = 24$ $6 \times 2 = 12$	$6 \times 5 = 30$ $6 \times 1 = 6$
III. Ability Enhancement Courses 1. Ability Enhancement Compulsory (2 Papers of 2 credit each) Environmental Studies English/MIL Communication 2. Ability Enhancement Elective (Skill Based) (4 Papers of 2 credit each)	$2 \times 4 = 8$ $4 \times 4 = 16$	$2 \times 4 = 8$ $4 \times 4 = 16$
Total	132	132

***Core and DSE courses without practical will have tutorial and have credit distribution of : 5 credits for theory and 1 credit for tutorial, total 6 credits, same as the papers with practical**

Structure of B.Sc. Regular Programme

Semester	Type	Core	AECC	SEC	DSE
	Credits	12 × 6 = 72	2 × 4 = 8	4 × 4 = 16	6 × 6 = 36
I		XXX-RC-1016	ENG-AE-1014/		
		CHE-RC-1016	ASM- AE-1014		
		ZZZ-RC-1016			
II		XXX-RC-2016	ENV-AE-2014		
		CHE-RC-2016			
		ZZZ-RC-2016			
III		XXX-RC-3016		XXX-SE-3YY4*	
		CHE-RC-3016			
		ZZZ-RC-3016			
IV		XXX-RC-4016		XXX-SE-4XX4*	
		CHE-RC-4016			
		ZZZ-RC-4016			
V			XXX-SE-5XX4*	XXX-RE-5XX6	
				CHE-RE-5YY6†	
				ZZZ-RE-5XX6	
VI			XXX-SE-6XX4*	XXX-RE-6XX6	
				CHE-RE-6YY4†	
				ZZZ-RE-6XX6	

Scheme for Choice Based Credit System in B. Sc. with Chemistry.

SEMESTER	COURSE OPTED	COURSE NAME	Credits
I	ENG-AE-1014/ASM- AE-1014	English/MIL communications	4
	XXX-RC-1016	DSC 1A	6
	CHE-RC-1016	CHEMISTRY1 Atomic Structure, Bonding, General Organic Chemistry & Aliphatic Hydrocarbons	4+2=6
		Lab- CHEMISTRY1	
	ZZZ-RC-1016	DSC 3A	6
Total Credits in Semester I			22
II	ENV-AE-2014	Environmental Studies	4
	XXX-RC-2016	DSC 1B	6
	CHE-RC-2016	CHEMISTRY2- <i>s</i> - and <i>p</i> -Block Elements, Transition Elements, Coordination Chemistry States of Matter & Chemical Kinetics	4+2=6
		Lab- CHEMISTRY2	
	ZZZ-RC-2016	DSC 3B	6
Total Credits in Semester II			22
III	XXX-RC-3016	DSC 1C	6
	CHE-RC-3016	CHEMISTRY3 Chemical Energetics, Equilibria & Functional Group Organic Chemistry-I	4+2=6
		Lab- CHEMISTRY3	
	ZZZ-RC-3016	DSC 3C	6
	XXX-SE-3YY4*	SEC-1	4
Total Credits in Semester III			22
IV	XXX-RC-4016	DSC 1D	6
	CHE-RC-4016	CHEMISTRY4 Solutions, Phase Equilibrium, Conductance, Electrochemistry & Functional Group Organic Chemistry-II	4+2=6
		Lab- CHEMISTRY4	
	ZZZ-RC-4016	DSC 3D	6
	XXX-SE-4XX4*	SEC-2	4
Total Credits in Semester IV			22
V	XXX-SE-5XX4*	SEC-3	4
	XXX-RE-5XX6	DSE-1A	6
	CHE-RE-5YY6†	DSE-2A	6
		Lab- DSE-2A	
	ZZZ-RE-5XX6	DSE-3A	6
Total Credits in Semester V			22
VI	XXX-SE-6XX4*	SEC-4	4
	XXX-RE-6XX6	DSE-1B	6
	CHE-RE-6YY6†	DSE-2B	6
		Lab-DSE-2B	
	ZZZ-RE-6XX6	DSE-3B	6
Total Credits in Semester VI			22

Grand Total Credits	132
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Core courses for B. Sc. with Chemistry (Credit: 06 each) /Chemistry as Generic Elective for other disciplines (Credit: 06 each)

CHE-RC/HG-1016. CHEMISTRY1: Atomic Structure, Bonding, General Organic Chemistry & Aliphatic Hydrocarbons (4) + Lab (2)

CHE-RC/HG-2016. CHEMISTRY2: *s*- and *p*-Block Elements, Transition Elements, Coordination Chemistry States of Matter & Chemical Kinetics (4) + Lab (2)

CHE-RC/HG-3016. CHEMISTRY3: Chemical Energetics, Equilibria & Functional Group Organic Chemistry-I (4) + Lab (2)

CHE-RC/HG-4016. CHEMISTRY4: Solutions, Phase Equilibrium, Conductance, Electrochemistry & Functional Group Organic Chemistry-II (4) + Lab (2)

† **Discipline Specific Elective Papers: (Credit: 06 each) (2 papers to be selected)- DSE 1-2**

DSE for Semester V

DSE-1(Any One from the following)

1. **CHE-RE-5016.** Applications of Computers in Chemistry (4) + Lab (2)
2. **CHE-RE-5026.** Analytical Methods in Chemistry (4) + Lab (2)
3. **CHE-RE-5036.** Molecular Modelling & Drug Design (4) + Lab (2)
4. **CHE-RE-5046.** Novel Inorganic Solids (4) + Lab (2)
5. **CHE-RE-5056.** Polymer Chemistry (4) + Lab (2)
6. **CHE-RE-5066.** Instrumental Methods of Analysis (4) + Lab (2)

DSE for Semester VI

DSE-2(Any One from the following)

7. **CHE-RE-6016.** Green Chemistry (4) + Lab (2)
8. **CHE-RE-6026.** Industrial Chemicals & Environment (4) + Lab (2)
9. **CHE-RE-6036.** Inorganic Materials of Industrial Importance (4) + Lab (2)
10. **CHE-RE-6046.** Research Methodology for Chemistry (5) + Tutorials (1)
11. **CHE-RE-6056.** Dissertation (6)

*** Skill Enhancement Courses (04 papers) (Credit: 04 each)- SEC1 to SEC4
(Students may choose SEC papers from same or different disciplines)**

SEC for Semester III

Any One from the following

1. **AAA-SE-3014:** English (Syllabus will be available on the GU website)
2. **CHE-SE-3024:** IT Skills for Chemists
3. **CHE-SE-3034:** Basic Analytical Chemistry

SEC for Semester IV

Any One from the following

4. **CHE-SE-4014:** Analytical Clinical Biochemistry
5. **CHE-SE-4024:** Green Methods in Chemistry
6. **CHE-SE-4034:** Pharmaceutical Chemistry

SEC for Semester V

Any One from the following

7. **CHE-SE-5014:** Chemical Technology & Society
8. **CHE-SE-5024:** Chemoinformatics

9. CHE-SE-5034: Business Skills for Chemists
10. CHE-SE-5044: Intellectual Property Rights

SEC for Semester VI

Any One from the following

11. CHE-SE-6014: Chemistry of Cosmetics & Perfumes
12. CHE-SE-6024: Pesticide Chemistry
13. CHE-SE-6034: Fuel Chemistry

Ability Enhancement Compulsory Courses (02 papers) (Credit: 04 each)- AECC1 to AECC2

AECC for Semester I

1. ENG-AE-1014: English Communications (<https://sites.google.com/a/gauhati.ac.in/syllabus-ug-cbcs/aecc/english-a>)

AECC for Semester II

2. ENV-AE-2014: Environmental Studies

Core courses for B. Sc. with Chemistry /Chemistry as Generic Elective

Semester I

CHE-RC/HG-1016: CHEMISTRY1

ATOMIC STRUCTURE, BONDING, GENERAL ORGANIC CHEMISTRY & ALIPHATIC HYDROCARBONS

(Credits: Theory-04, Lab-02)

Theory: 60 Lectures

Course Objective: This course may be divided into two broad parts-inorganic and organic chemistry. In inorganic chemistry part the students will be taught atomic structure, chemical bonding and molecular structure. The organic chemistry part contains fundamentals of organic chemistry, stereochemistry and aliphatic hydrocarbons.

Learning Outcome: After completion of this course the students will learn the atomic structure through the basic concepts of quantum mechanics. They will understand the chemical bonding through VB and MO approaches. In organic part, the students are

expected to learn basic ideas used in organic chemistry, stereochemistry, functional groups, alkanes, alkenes, alkynes etc.

Section A: Inorganic Chemistry-1 (30 Periods)

Atomic Structure: Review of: Bohr's theory and its limitations, dual behaviour of matter and radiation, de-Broglie's relation, Heisenberg Uncertainty principle. Hydrogen atom spectra. Need of a new approach to Atomic structure.

What is Quantum mechanics? Time independent Schrodinger equation and meaning of various terms in it. Significance of ψ and ψ^2 , Schrödinger equation for hydrogen atom. Radial and angular parts of the hydrogenic wavefunctions (atomic orbitals) and their variations for 1s, 2s, 2p, 3s, 3p and 3d orbitals (Only graphical representation). Radial and angular nodes and their significance. Radial distribution functions and the concept of the most probable distance with special reference to 1s and 2s atomic orbitals. Significance of quantum numbers, orbital angular momentum and quantum numbers m_l and m_s . Shapes of *s*, *p* and *d* atomic orbitals, nodal planes. Discovery of spin, spin quantum number (*s*) and magnetic spin quantum number (m_s).

Rules for filling electrons in various orbitals, Electronic configurations of the atoms. 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 bonding. Energy considerations in ionic bonding, lattice energy and solvation energy and their importance in the context of stability and solubility of ionic compounds. Statement of Born-Landé equation for calculation of lattice energy, Born-Haber cycle and its applications, polarizing power and polarizability. Fajan's rules, ionic character in covalent compounds, bond moment, dipole moment and percentage ionic character.

Covalent bonding: VB Approach: Shapes of some inorganic molecules and ions on the basis of VSEPR and hybridization with suitable examples of linear, trigonal planar, square planar, tetrahedral, trigonal bipyramidal and octahedral arrangements.

Concept of resonance and resonating structures in various inorganic and organic compounds. 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, NO and NO⁺. Comparison of VB and MO approaches.

(16 Lectures)

Section B: Organic Chemistry-1 (30 Periods)

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 (Partial catalytic hydrogenation) and *trans* alkenes (Birch reduction). *Reactions:* *cis*-addition (alk. KMnO₄) 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 CaC₂ 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 KMnO₄, ozonolysis and oxidation with hot alk. KMnO₄.

(12 Lectures)

Recommended Books:

1. J. D. Lee: *A new Concise Inorganic Chemistry*, E L. B. S.
2. F. A. Cotton & G. Wilkinson: *Basic Inorganic Chemistry*, John Wiley.
3. Douglas, McDaniel and Alexader: *Concepts and Models in Inorganic Chemistry*, John Wiley.
4. James E. Huheey, Ellen Keiter and Richard Keiter: *Inorganic Chemistry: Principles of Structure and Reactivity*, Pearson Publication.
5. T. W. Graham Solomon: *Organic Chemistry*, John Wiley and Sons.
6. Peter Sykes: *A Guide Book to Mechanism in Organic Chemistry*, Orient Longman.
7. E. L. Eliel: *Stereochemistry of Carbon Compounds*, Tata McGraw Hill.
8. I. L. Finar: *Organic Chemistry* (Vol. I & II), E. L. B. S.
9. R. T. Morrison & R. N. Boyd: *Organic Chemistry*, Prentice Hall.
10. Arun Bahl and B. S. Bahl: *Advanced Organic Chemistry*, S. Chand

LAB: CHEMISTRY1

ATOMIC STRUCTURE, BONDING, GENERAL ORGANIC CHEMISTRY & ALIPHATIC HYDROCARBONS

60 Lectures

Section A: Inorganic Chemistry - Volumetric Analysis

1. Estimation of sodium carbonate and sodium hydrogen carbonate present in a mixture.
2. Estimation of oxalic acid by titrating it with KMnO_4 .
3. Estimation of water of crystallization in Mohr's salt by titrating with KMnO_4 .
4. Estimation of Fe (II) ions by titrating it with $\text{K}_2\text{Cr}_2\text{O}_7$ using internal indicator.
5. Estimation of Cu (II) ions iodometrically using $\text{Na}_2\text{S}_2\text{O}_3$.

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: Measure the R_f value in each case (combination of two compounds to be given)
 - (a) Identify and separate the components of a given mixture of 2 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.

Recommended Books:

1. Vogel's Qualitative Inorganic Analysis, A.I. Vogel, Prentice Hall, 7th Edition.
 2. Vogel's Quantitative Chemical Analysis, A.I. Vogel, Prentice Hall, 6th Edition.
 3. Textbook of Practical Organic Chemistry, A.I. Vogel, Prentice Hall, 5th edition.
 4. Practical Organic Chemistry, F. G. Mann. & B. C. Saunders, Orient Longman, 1960.
-

Semester II

CHE-RC/HG-2016: CHEMISTRY2

s- AND *p*-BLOCK ELEMENTS, TRANSITION ELEMENTS, COORDINATION CHEMISTRY STATES OF MATTER & CHEMICAL KINETICS

(Credits: Theory-04, Lab-02)

Theory: 60 Lectures

Course Objective: This course may be divided into two broad parts-inorganic and physical chemistry. Three units-main group elements, transition elements and co-ordination chemistry will be taught in the inorganic chemistry part. The physical chemistry part contains states of matter and chemical kinetics.

Learning Outcome: After completion of this course the students will learn periodic properties in main group elements, transition metals (3d series). They will also learn the crystal field theory in coordination chemistry unit. In physical chemistry part, the students are expected to learn kinetic theory of gases, ideal gas and real gases, surface tension, viscosity, basic solid state chemistry and chemical kinetics.

s- and p-Block Elements

Periodicity in s- and p-block elements with respect to electronic configuration, atomic and ionic size, ionization enthalpy, electronegativity (Pauling, Mulliken, and Alfred-Rochow scales). Allotropy in C, S, and P.

Oxidation states with reference to elements in unusual and rare oxidation states like carbides and nitrides), inert pair effect, diagonal relationship and anomalous behaviour of first member of each group.

(10 Lectures)

Transition Elements (3d series)

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

(6Lectures)

Coordination Chemistry

Coordination compounds, types of ligands, Werner's theory, IUPAC nomenclature and isomerism in coordination compounds. Stereochemistry of complexes with 4 and 6 coordination numbers.

Drawbacks of VBT. 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 D. Spectrochemical series. Comparison of CFSE for *Oh* and *Td* complexes, Tetragonal distortion of octahedral geometry. Jahn-Teller distortion, Square planar coordination.

(14 Lectures)

Section B: Physical Chemistry-3 (30 Lectures)

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 CO₂.

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:

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

LAB: CHEMISTRY2

s- AND *p*-BLOCK ELEMENTS, TRANSITION ELEMENTS, COORDINATION CHEMISTRY STATES OF MATTER & CHEMICAL KINETICS 60 Lectures

Section A: Inorganic Chemistry

Semi-micro qualitative analysis using H₂S of mixtures - not more than four ionic species (two anions and two cations and excluding insoluble salts) out of the following:

CO₃²⁻, NO₂⁻, S²⁻, SO₃²⁻, S₂O₃²⁻, CH₃COO⁻, F⁻, Cl⁻, Br⁻, I⁻, NO₃⁻, BO₃³⁻, C₂O₄²⁻, PO₄³⁻, NH₄⁺, K⁺, Pb²⁺, Cu²⁺, Cd²⁺, Bi³⁺, Sn²⁺, Sb³⁺, Fe³⁺, Al³⁺, Cr³⁺, Zn²⁺, Mn²⁺, Co²⁺, Ni²⁺, Ba²⁺, Sr²⁺, Ca²⁺, Mg²⁺

(Spot tests should be carried out wherever feasible)

1. Estimate the amount of nickel present in a given solution as bis(dimethylglyoximate) nickel(II) or aluminium as oximate in a given solution gravimetrically.

2. Draw calibration curve (absorbance at λ_{max} vs. concentration) for various concentrations of a given coloured compound ($\text{KMnO}_4/\text{CuSO}_4$) and estimate the concentration of the same in a given solution.
3. Determine the composition of the Fe^{3+} -salicylic acid complex solution by Job's method.
4. Estimation of (i) Mg^{2+} or (ii) Zn^{2+} by complexometric titrations using EDTA.
5. Estimation of total hardness of a given sample of water by complexometric titration.
6. Determination of concentration of Na^+ and K^+ using Flame Photometry.

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.
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.
 - c. Compare the strengths of HCl and H_2SO_4 by studying kinetics of hydrolysis of methyl acetate

Reference Books:

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

Semester III

CHE-RC/HG-3016: CHEMISTRY 3

CHEMICAL ENERGETICS, EQUILIBRIA & FUNCTIONAL ORGANIC CHEMISTRY-I

(Credits: Theory-04, Lab-02)

Theory: 60 Lectures

Course Objective: This course contains two broad parts- physical and organic chemistry. In physical chemistry part the students will be taught chemical energetics,

chemical equilibrium and ionic equilibrium. In organic chemistry part, the students will be introduced to different classes of organic compounds.

Learning Outcome: After completion of this course the students will be able to understand the chemical system from thermodynamic points of view. They will also learn two very important topics in chemistry- chemical equilibrium and ionic equilibrium. In organic chemistry part, the students are expected to learn various classes of organic molecules-alkyl halides, aryl halides, alcohols, phenols, ethers, aldehydes and ketones.

Section A: Physical Chemistry-1 (30 Lectures)

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° , Le Chatelier's principle. Relationships between K_p , K_c and K_x 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 Lectures)

Section B: Organic Chemistry-2 (30 Lectures)

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

Aromatic hydrocarbons

Preparation (Case benzene): from phenol, by decarboxylation, from acetylene, from benzene sulphonic acid.

Reactions: (Case 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 case): from phenol, Sandmeyer & Gattermann reactions.

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

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 $^\circ$, 2 $^\circ$ and 3 $^\circ$ alcohols: using Grignard reagent, Ester hydrolysis, Reduction of aldehydes, ketones, carboxylic acid 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: (Phenol case) *Preparation:* Cumene hydroperoxide method, from diazonium salts.

Reactions: Electrophilic substitution: Nitration, halogenation and sulphonation. Reimer-Tiemann Reaction, Gattermann-Koch Reaction, Houben-Hoesch Condensation, Schotten – Baumann Reaction.

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

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

Preparation: from acid chlorides and from 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-Ponndorf Verley reduction.

(14 Lectures)

Recommended Books:

1. T. W. Graham Solomons: *Organic Chemistry, John Wiley and Sons.*
2. Peter Sykes: *A Guide Book to Mechanism in Organic Chemistry*, Orient Longman.
3. I.L. Finar: *Organic Chemistry* (Vol. I & II), E. L. B. S.
4. R. T. Morrison & R. N. Boyd: *Organic Chemistry*, Prentice Hall.
5. Arun Bahl and B. S. Bahl: *Advanced Organic Chemistry*, S. Chand.
6. G. M. Barrow: *Physical Chemistry* Tata McGraw-Hill (2007).

7. G. W. Castellan: *Physical Chemistry* 4th Edn. Narosa (2004).
 8. J. C. Kotz, P. M. Treichel & J. R. Townsend: *General Chemistry* Cengage Learning India Pvt. Ltd., New Delhi (2009).
 9. B. H. Mahan: *University Chemistry* 3rd Ed. Narosa (1998).
 10. R. H. Petrucci: *General Chemistry* 5th Ed. Macmillan Publishing Co.: New York (1985).
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LAB: CHEMISTRY3

CHEMICAL ENERGETICS, EQUILIBRIA & FUNCTIONAL ORGANIC CHEMISTRY-I 60 Lectures

Section A: Physical Chemistry

Thermochemistry

1. Determination of heat capacity of calorimeter for different volumes.
2. Determination of enthalpy of neutralization of hydrochloric acid with sodium hydroxide.
3. Determination of enthalpy of ionization of acetic acid.
4. Determination of integral enthalpy of solution of salts (KNO₃, NH₄Cl).
5. Determination of enthalpy of hydration of copper sulphate.
6. Study of the solubility of benzoic acid in water and determination of ΔH .

Ionic equilibria

pH measurements

- a) 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.
- b) 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

Recommended Books

1. A.I. Vogel: Textbook of Practical Organic Chemistry, 5th edition, Prentice-Hall.
2. F. G. Mann & B. C. Saunders, Practical Organic Chemistry, Orient Longman (1960).
3. B.D. Khosla, Senior Practical Physical Chemistry, R. Chand & Co.

Semester IV

CHE- RC/HG-4016: CHEMISTRY4

SOLUTIONS, PHASE EQUILIBRIUM, CONDUCTANCE, ELECTROCHEMISTRY & FUNCTIONAL GROUP ORGANIC CHEMISTRY

(Credits: Theory-04, Lab-02)

Theory: 60 Lectures

***Course Objective:** This course may be divided into two broad parts-physical and organic chemistry. In 1st part of this course students will be introduced to solutions, phase equilibrium and electrochemistry. The 2nd part contains carboxylic acid and derivatives, amines and diazonium salt and biochemistry.*

***Learning Outcome:** After completion of this course the students learn solutions, phase rule and its application in specific cases, basics of conductance and electrochemistry. Students will also learn some important topics of organic and biochemistry- carboxylic acids, amines, amino acids, peptides, proteins and carbohydrates.*

Section A: Physical Chemistry-2 (30 Lectures)

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.

Azeotropes. Partial miscibility of liquids: Critical solution temperature; effect of impurity on partial miscibility of liquids. Immiscibility of liquids- Principle of steam distillation. Nernst distribution law and its applications, solvent extraction.

Phase Equilibrium

Phases, components and degrees of freedom of a system, criteria of phase equilibrium. Gibbs Phase 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, congruent and incongruent melting points (lead-silver, FeCl₃-H₂O and Na-K only).

Conductance

Conductivity, equivalent and molar conductivity and their variation with dilution for weak and 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 acidbase).

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).

Section B: Organic Chemistry-3 (30 Lectures)

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 – Vohlard - Zelinsky Reaction.

Carboxylic acid derivatives (aliphatic): (Upto 5 carbons)

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

Reactions: Comparative study of nucleophilicity 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's Phthalimide synthesis, Hofmann Bromamide reaction.

Reactions: Hofmann vs. Saytzeff elimination, Carbylamine test, Hinsberg test, with HNO_2 , Schotten – Baumann Reaction. Electrophilic substitution (case 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's phthalimide synthesis. Zwitterion, Isoelectric point and Electrophoresis.

Reactions of Amino acids: ester of –COOH group, acetylation of –NH₂ group, complexation with Cu₂₊ ions, ninhydrin test.

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

Determination of Primary structure of Peptides by degradation Edmann degradation (Nterminal) and C-terminal (thiohydantoin and with carboxypeptidase enzyme). Synthesis of simple peptides (upto dipeptides) by N-protection (t-butyloxycarbonyl and phthaloyl) & Cactivating 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)

Recommended Books:

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

LAB: CHEMISTRY4

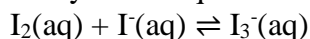
**SOLUTIONS, PHASE EQUILIBRIUM, CONDUCTANCE, ELECTROCHEMISTRY
& FUNCTIONAL ORGANIC CHEMISTR-II**

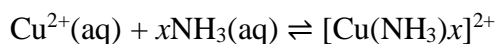
60 Lectures

Section A: Physical Chemistry

Distribution

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





Phase equilibria

- Construction of the phase diagram of a binary system (simple eutectic) using cooling curves.
- Determination of the critical solution temperature and composition of the phenol water system and study of the effect of impurities on it.
- Study of the variation of mutual solubility temperature with concentration for the phenol water system and determination of the critical solubility temperature.

Conductance

- Determination of cell constant
- Determination of equivalent conductance, degree of dissociation and dissociation constant of a weak acid.
- Perform the following conductometric titrations:
 - Strong acid vs. strong base
 - Weak acid vs. strong base

Potentiometry

Perform the following potentiometric titrations:

- Strong acid vs. strong base
- Weak acid vs. strong base
- 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, nitro, amines) and preparation of one derivative.

II

- Separation of amino acids by paper chromatography
- Determination of the concentration of glycine solution by formylation method.
- Titration curve of glycine
- Action of salivary amylase on starch
- Effect of temperature on the action of salivary amylase on starch.
- Determination of the saponification value of an oil/fat.
- Determination of the iodine value of an oil/fat
- Differentiation between a reducing/nonreducing sugar.
- Extraction of DNA from onion/ cauliflower

Recommended Books:

- A.I. Vogel: Textbook of Practical Organic Chemistry, Prentice Hall, 5th Edn.
 - F. G. Mann & B. C. Saunders: Practical Organic Chemistry, Orient Longman, 1960.
 - B.D. Khosla: Senior Practical Physical Chemistry, R. Chand & Co.
 - Ahluwalia, V.K. & Aggarwal, R. *Comprehensive Practical Organic Chemistry*, Universities Press.
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Discipline Specific Elective (DSE)

CHE-RE-5016: APPLICATIONS OF COMPUTERS IN CHEMISTRY

(Credits: Theory-04, Lab-02)

Theory: 60 Lectures

Course Objective: This course intends to make learners familiar with basics of computer language, computer programming, handling of experimental data, curve fitting etc to analyze experimental results. This basic knowledge will help the students to perform and interpret results of various chemistry practicals.

Learning Outcome: After the completion of this course it will help the student to interpret laboratory data, curve fitting of experimental work, also perform quantum mechanical calculations for various molecular models.

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.

Recommended Books:

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

60 Lectures

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.

Recommended Books:

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

CHE-RE-5026: ANALYTICAL METHODS IN CHEMISTRY

(Credits: Theory-04, Lab -02)

Theory: 60 Lectures

Course Objective: *This is an elective course designed to complement the needs of students who wish to learn more about the qualitative/quantitative characterization and separation techniques. The content of this course aims to cover some of the widely used instrumental techniques for characterization of samples. Experiments included aim at giving students hands on experience using different instrumental techniques and chemical analysis.*

Learning outcome: *On successful completion students will have theoretical understanding about choice of various analytical techniques used for qualitative and quantitative characterization of samples. At the same time through the experiments students will gain hands on experience of the discussed techniques. This will enable students to take judicious decisions while analyzing different samples.*

Qualitative and quantitative aspects of analysis:

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

(5 Lectures)

Optical methods of analysis:

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

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

Infrared Spectroscopy: Basic principles of instrumentation (choice of source, monochromator & detector) for continuous wave and Fourier transform spectrometers; sampling techniques.

Structure elucidation through interpretation of data. Effect and importance of isotope substitution.

Flame Atomic Absorption and Emission Spectrometry: Basic principles of instrumentation (choice of source, monochromator, and 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.

(25 Lectures)

Thermal methods of analysis:

Theory of thermogravimetry (TG), basic principle of instrumentation. Techniques for quantitative estimation of Ca and Mg from their mixture.

(5 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 pK_a values.

(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, calculation of Enantiomeric excess (ee)/ diastereomeric excess (de) ratios and determination of enantiomeric composition using NMR, Chiral solvents and chiral shift reagents. Chiral chromatographic techniques using chiral columns (GC and HPLC).

Role of computers in instrumental methods of analysis.

(15 Lectures)

Recommended Books:

1. Mendham, J. et al.: Vogel's Text Book of Quantitative Chemical Analysis ; 6th Ed. Pearson Education, 2009.
 2. Willard, Hobert H. et al.: Instrumental Methods of Analysis, 7th Ed. CBS Publishers & Distributors, 2004.
 3. Christian, Gary D: Analytical Chemistry, 6th Ed. Wiley India (P) Ltd., 2004.
 4. Harris, Daniel C: Exploring Chemical Analysis, 4th Ed. W. H. Freeman, 2008.
 5. Khopkar, S.M.: Basic Concepts of Analytical Chemistry, 3rd Ed. New Age, International Publisher, 2009.
 6. Skoog, D.A. Holler F.J. and Nieman, T.A. Principles of Instrumental Analysis, 6th Ed. Thomson Asia Pvt. Ltd. Singapore.
 7. Mikes, O. and Chalmes, R.A. Laboratory Hand Book of Chromatographic & Allied Methods, Elles Harwood Ltd. London.1979
 8. Ditts, R.V. *Analytical Chemistry: Methods of separation.* Van Nostrand, New York, 1974.
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LAB: ANALYTICAL METHODS IN CHEMISTRY

60 Lectures

1. Separation Techniques

I. Chromatography:

(a) Separation of mixtures

(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 R_f values.

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

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

II. Solvent Extractions:

(i) 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.

(ii) Solvent extraction of zirconium with amberliti LA-1, separation from a mixture of irons and gallium.

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

4. Determination of Na, Ca, Li in cola drinks and fruit juices using flame photometric techniques.

5. Analysis of soil:

(i) Determination of pH of soil.

(ii) Total soluble salt

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

6. Ion exchange:

(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.

7. Spectrophotometry

(i) Determination of pKa values of indicator using spectrophotometry.

(ii) Structural characterization of compounds by infrared spectroscopy.

(iii) Determination of dissolved oxygen in water.

(iv) Determination of chemical oxygen demand (COD).

(v) Determination of Biological oxygen demand (BOD).

(vi) Determine the composition of the Ferric-salicylate/ ferric-thiocyanate complex by

Job's method.

Recommended Books:

1. Vogel, Arthur I: A Test book of Quantitative Inorganic Analysis (Rev. by G.H. Jeffery and others) 5th Ed. The English Language Book Society of Longman .
2. Willard, Hobert H. et al.: Instrumental Methods of Analysis, 7th Ed. Wardsworth Publishing Company, Belmont, California, USA, 1988.
3. Christian, Gary D; Analytical Chemistry, 6th Ed. John Wiley & Sons, New York, 2004.
4. Harris, Daniel C: Exploring Chemical Analysis, Ed. New York, W.H. Freeman, 2001.
5. Khopkar, S.M. Basic Concepts of Analytical Chemistry. New Age, International Publisher, 2009.
6. Skoog, D.A. Holler F.J. and Nieman, T.A. Principles of Instrumental Analysis, Thomson Asia Pvt. Ltd. Singapore.
7. Mikes, O. & Chalmes, R.A. Laboratory Hand Book of Chromatographic & Allied Methods, Elles Harwood Ltd. London.
9. Ditts, R.V. *Analytical Chemistry: Methods of separation*. Van Nostrand, New York, 1974.

CHE-RE-5036: MOLECULAR MODELLING & DRUG DESIGN

(Credits: Theory-04, Lab-02)

Theory: 60 Lectures

Course Objective: The course introduces students to the basic principles of computer assisted drug design, modelling and the important theoretical concepts and programming.

Learning Outcome: Students will be able to identify basic components of computer and programming as applied to computer assisted design and modelling of molecules.

Introduction to Molecular Modelling:

Introduction. Useful Concepts in Molecular Modelling: Coordinate Systems. Potential Energy Surfaces. Molecular Graphics. Surfaces. Computer Hardware and Software. The Molecular Modelling Literature.

(10 Lectures)

Force Fields:

Fields. Bond Stretching. Angle Bending. Introduction to nonbonded interactions. Electrostatic interactions. van der Waals Interactions. Hydrogen bonding in Molecular Mechanics. Force Field Models for the Simulation of Liquid Water.

(14 Lectures)

Energy Minimization and Computer Simulation:

Minimization and related methods for exploring the energy surface. Non-derivative method, First and second order minimization methods. Computer simulation methods. Simple

thermodynamic properties and Phase Space. Boundaries. Analyzing the results of a simulation and estimating Errors.

(12 Lectures)

Molecular Dynamics & Monte Carlo Simulation:

Molecular Dynamics Simulation Methods. Molecular Dynamics using simple models. Molecular Dynamics with continuous potentials. Molecular Dynamics at constant temperature and pressure. Metropolis method. Monte Carlo simulation of molecules. Models used in Monte Carlo simulations of polymers.

(12 Lectures)

Structure Prediction and Drug Design:

Structure prediction - Introduction to comparative Modeling. Sequence alignment. Constructing and evaluating a comparative model. Predicting protein structures by 'Threading', Molecular docking. Structure based de novo ligand design,

Drug Discovery – Chemoinformatics – QSAR.

(12 Lectures)

Recommended Books:

1. A.R. Leach, Molecular Modelling Principles and Application, Longman, 2001.
 2. J.M. Haile, Molecular Dynamics Simulation Elementary Methods, John Wiley and Sons, 1997.
 3. Satya Prakash Gupta, QSAR and Molecular Modeling, Springer - Anamaya Publishers, 2008.
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LAB: MOLECULA MODELLING & DRUG DESIGN

60 Lectures

- i. Compare the optimized C-C bond lengths in ethane, ethene, ethyne and benzene. Visualize the molecular orbitals of the ethane σ bonds and ethene, ethyne, benzene and pyridine π bonds.
- ii. (a) Perform a conformational analysis of butane. (b) Determine the enthalpy of isomerization of *cis* and *trans* 2-butene.
- iii. Visualize the electron density and electrostatic potential maps for LiH, HF, N₂, NO and CO and comment. Relate to the dipole moments. Animate the vibrations of these molecules.
- iv. (a) Relate the charge on the hydrogen atom in hydrogen halides with their acid character. (b) Compare the basicities of the nitrogen atoms in ammonia, methylamine, dimethylamine and trimethylamine.
- v. (a) Compare the shapes of the molecules: 1-butanol, 2-butanol, 2-methyl-1-propanol, and 2-methyl-2-propanol. Note the dipole moment of each molecule. (b) Show how the shapes affect the trend in boiling points: (118 °C, 100 °C, 108 °C, 82 °C, respectively).
- vi. Build and minimize organic compounds of your choice containing the following functional groups. Note the dipole moment of each compound: (a) alkyl halide (b) aldehyde (c) ketone (d) amine (e) ether (f) nitrile (g) thiol (h) carboxylic acid (i) ester (j) amide.

- vii. (a) Determine the heat of hydration of ethylene. (b) Compute the resonance energy of benzene by comparison of its enthalpy of hydrogenation with that of cyclohexene.
- viii. Arrange 1-hexene, 2-methyl-2-pentene, (*E*)-3-methyl-2-pentene, (*Z*)-3-methyl-2-pentene, and 2,3-dimethyl-2-butene in order of increasing stability.
- ix. (a) Compare the optimized bond angles H₂O, H₂S, H₂Se. (b) Compare the HAH bond angles for the second row dihydrides and compare with the results from qualitative MO theory.

Note: Software: ChemSketch, ArgusLab (www.planaria-software.com), TINKER 6.2 (dasher.wustl.edu/ffe), WebLab Viewer, Hyperchem, or any similar software.

Recommended Books:

1. A.R. Leach, Molecular Modelling Principles and Application, Longman, 2001.
 2. J.M. Haile, Molecular Dynamics Simulation Elementary Methods, John Wiley and Sons, 1997.
 3. Satya Prakash Gupta, QSAR and Molecular Modeling, Springer - Anamaya Publishers, 2008.
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CHE-RE-5046: NOVEL INORGANIC SOLIDS

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Course Objective: This introductory course intends to make learners familiar with a wide variety of technologically important and emerging materials. It will prepare the learners for studying materials further at the master's level. Prior completion of one introductory UG level course on inorganic and physical chemistry will be essential.

Learning outcome: After the completion of this course it will also be possible for the students to opt for studying an interdisciplinary master's programme with an emphasis on the synthesis and applications of various materials or take up a job in the materials production and/or processing industry.

Synthesis and modification of inorganic solids:

Conventional heat and beat methods, Co-precipitation method, Sol-gel methods, Hydrothermal method, Ion-exchange and Intercalation methods.

(10 Lectures)

Inorganic solids of technological importance:

Solid electrolytes – Cationic, anionic, mixed Inorganic pigments – coloured solids, white and black pigments.

Molecular material and fullerides, molecular materials & chemistry – one-dimensional metals, molecular magnets, metal containing liquid crystals.

(10 Lectures)

Nanomaterials:

Overview of nanostructures and nanomaterials: classification.

Preparation of gold and silver metallic nanoparticles, self-assembled nanostructures-control of nanoarchitecture-one dimensional control. Carbon nanotubes and inorganic nanowires.

Bio-inorganic nanomaterials, DNA and nanomaterials, natural and artificial nanomaterials, bionano composites.

(10 Lectures)

Introduction to engineering materials for mechanical construction:

Composition, mechanical and fabricating characteristics and applications of various types of cast irons, plain carbon and alloy steels, copper, aluminium and their alloys like duralumin, brasses and bronzes cutting tool materials, super alloys thermoplastics, thermosets and composite materials.

(10 Lectures)

Composite materials:

Introduction, limitations of conventional engineering materials, role of matrix in composites, classification, matrix materials, reinforcements, metal-matrix composites, polymer-matrix composites, fibre-reinforced composites, environmental effects on composites, applications of composites.

(10 Lectures)

Speciality polymers:

Ceramics & Refractory: Introduction, classification, properties, raw materials, manufacturing and applications.

(10 Lectures)

Recommended Books:

1. Shriver & Atkins. Inorganic Chemistry, Peter Atkins, Tina Overton, Jonathan Rourke, Mark Weller and Fraser Armstrong, 5th Edition, Oxford University Press (2011-2012)
2. Smart, L. E., Moore, E. A., Solid State Chemistry: An Introduction, 4th Ed., CRC Press, 2012.
3. Poole, C. P., Ovens, F. J., Introduction to Nanotechnology, Wiley India, 2009.
4. Murty, B. S., Shankar, P., Raj, B., Rath, B. B., Murday, J. Textbook of Nanoscience and Nanotechnology, Springer, 2013.

LAB: NOVEL INORGANIC SOLIDS

60 Lectures

1. Determination of cation exchange capacity.
2. Synthesis of oxides by ceramic method.
3. Synthesis of hydrogel by co-precipitation method.
4. Synthesis of silver and gold metal nanoparticles.

Recommended Book:

1. Fahlman, B. D., Materials *Chemistry*, Springer (2011).

CHE-RE-5056: POLYMER CHEMISTRY

(Credits: Theory-06, Lab-02)

Theory: 60 Lectures

***Course objective:** This is an introductory level course in polymer chemistry. The aim of the course is to introduce the theory and applications of polymer chemistry to the students. Some industrially important polymers and conducting polymers, a promising class of polymeric materials for next generation devices will also be introduced in this course.*

***Learning outcome:** After completion of this course the students will learn the definition and classifications of polymers, kinetics of polymerization, molecular weight of polymers, glass transition temperature, and polymer solutions etc. They also learn the brief introduction of preparation, structure and properties of some industrially important and technologically promising polymers.*

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 (M_n , M_w , 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 (T_g) and determination of T_g, Free volume theory,

WLF equation, Factors affecting glass transition temperature (T_g).

(8 Lectures)

Polymer Solution – Criteria for polymer solubility, Solubility parameter,

Thermodynamics of polymer solutions, entropy, enthalpy, and free energy change of mixing of polymer 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)

Recommended Books:

1. *Seymour's Polymer Chemistry*, Marcel Dekker, Inc.
 2. G. Odian: *Principles of Polymerization*, John Wiley.
 3. F.W. Billmeyer: *Text Book of Polymer Science*, John Wiley.
 4. P. Ghosh: *Polymer Science & Technology*, Tata Mcgraw-Hill.
 5. R.W. Lenz: *Organic Chemistry of Synthetic High Polymers*.
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LAB: POLYMER CHEMISTRY

60 Lectures

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-isobutyronitrile (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 propylidene (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.

Recommended Books:

1. Malcolm P. Stevens, Polymer Chemistry: An Introduction, 3rd Ed.
 2. Harry R. Allcock, Frederick W. Lampe and James E. Mark, Contemporary Polymer Chemistry, 3rd ed. Prentice-Hall (2003)
 3. Fred W. Billmeyer, Textbook of Polymer Science, 3rd ed. Wiley-Interscience (1984)
 4. Joel R. Fried, Polymer Science and Technology, 2nd ed. Prentice-Hall (2003)
 5. Petr Munk and Tejraj M. Aminabhavi, Introduction to Macromolecular Science, 2nd ed. John Wiley & Sons (2002)
 6. L. H. Sperling, Introduction to Physical Polymer Science, 4th ed. John Wiley & Sons (2005)
 7. Malcolm P. Stevens, Polymer Chemistry: An Introduction, 3rd ed. Oxford University Press (2005)
 8. Seymour/ Carraher's Polymer Chemistry, 9th ed. by Charles E. Carraher, Jr. (2013).
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CHE-RE-5066: INSTRUMENTAL METHODS OF CHEMICAL ANALYSIS

(Credits: Theory-04, Lab -02)

Theory: 60 Lectures

Course Objective: Students shall be introduced to the fundamental concepts/theory and application of different analytical techniques, as applied to chemistry.

Learning Outcome: Students shall be able to explain the theoretical basis of different analytical techniques, identify the experimental requirements and compare/analyze the data/results thereof.

Introduction to spectroscopic methods of analysis:

Recap of the spectroscopic methods covered in detail in the core chemistry syllabus: Treatment of analytical data, including error analysis. Classification of analytical methods and the types of instrumental methods. Consideration of electromagnetic radiation.

(4 Lectures)

Molecular spectroscopy:

Infrared spectroscopy:

Interactions with molecules: absorption and scattering. Means of excitation (light sources), separation of spectrum (wavelength dispersion, time resolution), detection of the signal (heat, differential detection), interpretation of spectrum (qualitative, mixtures, resolution), advantages of Fourier Transform (FTIR). Samples and results expected. Applications: Issues of quality assurance and quality control, Special problems for portable instrumentation and rapid detection.

UV-Visible/ Near IR – emission, absorption, fluorescence and photoacoustic. Excitation sources (lasers, time resolution), wavelength dispersion (gratings, prisms, interference filters, laser, placement of sample relative to dispersion, resolution), Detection of signal (photocells, photomultipliers, diode arrays, sensitivity and S/N), Single and Double Beam instruments, Interpretation (quantification, mixtures, absorption vs. fluorescence and the use of time, photoacoustic, fluorescent tags).

(16 Lectures)

Separation techniques

Chromatography: Gas chromatography, liquid chromatography, supercritical fluids, Importance of column technology (packing, capillaries), Separation based on increasing number of factors (volatility, solubility, interactions with stationary phase, size, electrical field), Detection: simple vs. specific (gas and liquid), Detection as a means of further analysis (use of tags and coupling to IR and MS), Electrophoresis (plates and capillary) and use with DNA analysis.

Immunoassays and DNA techniques

Mass spectroscopy: Making the gaseous molecule into an ion (electron impact, chemical ionization), Making liquids and solids into ions (electrospray, electrical discharge, laser desorption, fast atom bombardment), Separation of ions on basis of mass to charge ratio, Magnetic, Time of flight, Electric quadrupole. Resolution, time and multiple separations, Detection and interpretation (how this is linked to excitation).

(16 Lectures)

Elemental analysis:

Mass spectrometry (electrical discharges).

Atomic spectroscopy: Atomic absorption, Atomic emission, and Atomic fluorescence
Excitation and getting sample into gas phase (flames, electrical discharges, plasmas),
Wavelength separation and resolution (dependence on technique), Detection of radiation (simultaneous/scanning, signal noise), Interpretation (errors due to molecular and ionic species, matrix effects, other interferences).

(8 Lectures)

NMR spectroscopy: Principle, Instrumentation, Factors affecting chemical shift, Spincoupling, Applications.

(4 Lectures)

Electroanalytical Methods: Potentiometry & Voltammetry

(4 Lectures)

Radiochemical Methods

(4 Lectures)

X-ray analysis and electron spectroscopy (surface analysis)

(4 Lectures)

Recommended books:

1. Principles of Instrumental Analysis - 6th Edition by Douglas A. Skoog, F. James Holler, and Stanley Crouch (ISBN 0-495-01201-7).
 2. Instrumental Methods of Analysis, 7th ed, Willard, Merritt, Dean, Settle.
 3. P.W. Atkins: Physical Chemistry.
 4. G.W. Castellan: Physical Chemistry.
 5. C.N. Banwell: Fundamentals of Molecular Spectroscopy.
 6. Brian Smith: Infrared Spectral Interpretations: A Systematic Approach.
 7. W.J. Moore: Physical Chemistry.
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LAB: INSTRUMENTAL METHODS OF CHEMICAL ANALYSIS

60 Lectures

1. Safety Practices in the Chemistry Laboratory
2. Determination of the isoelectric pH of a protein.
3. Titration curve of an amino acid.
4. Determination of the void volume of a gel filtration column.
5. Determination of a Mixture of Cobalt and Nickel (UV/Vis spec.)
6. Study of Electronic Transitions in Organic Molecules (i.e., acetone in water)
7. IR Absorption Spectra (Study of Aldehydes and Ketones)
8. Determination of Calcium, Iron, and Copper in Food by Atomic Absorption
9. Quantitative Analysis of Mixtures by Gas Chromatography (i.e., chloroform and carbon tetrachloride)
10. Separation of Carbohydrates by HPLC
11. Determination of Caffeine in Beverages by HPLC
12. Potentiometric Titration of a Chloride-Iodide Mixture
13. Cyclic Voltammetry of the Ferrocyanide/Ferricyanide Couple
14. Nuclear Magnetic Resonance
15. Use of fluorescence to do "presumptive tests" to identify blood or other body fluids.
16. Use of "presumptive tests" for anthrax or cocaine
17. Collection, preservation, and control of blood evidence being used for DNA testing
18. Use of capillary electrophoresis with laser fluorescence detection for nuclear DNA (Y-chromosome only or multiple chromosome)
19. Use of sequencing for the analysis of mitochondrial DNA
20. Laboratory analysis to confirm anthrax or cocaine

21. Detection in the field and confirmation in the laboratory of flammable accelerants or explosives
22. Detection of illegal drugs or steroids in athletes
23. Detection of pollutants or illegal dumping
24. Fibre analysis

At least 10 experiments to be performed.

Recommended Books:

1. Principles of Instrumental Analysis - 6th Edition by Douglas A. Skoog, F. James Holler and Stanley Crouch (ISBN 0-495-01201-7).
2. Instrumental Methods of Analysis, 7th ed, Willard, Merritt, Dean, Settle.

CHE-RE-6016: GREEN CHEMISTRY

(Credits: Theory-04, Lab -02)

Theory: 60 Lectures

***Course Objective:** The learners will be taught about the emerging discipline of green chemistry particularly to differentiate as to how the principles of green chemistry may be applied to organic synthesis.*

***Learning Outcome:** Apart from introducing learners to the principles of green chemistry, this course will make them conversant with applications of green chemistry to organic synthesis. Students will be prepared for taking up entry level jobs in the chemical industry. They also will have the option of studying further in the area.*

Introduction to Green Chemistry

What is Green Chemistry? Need for Green Chemistry. Goals of Green Chemistry. Limitations/ Obstacles in the pursuit of the goals of Green Chemistry.

(4 Lectures)

Principles of Green Chemistry and Designing a Chemical synthesis

Twelve principles of Green Chemistry with their explanations and examples; Designing a Green Synthesis using these principles; Prevention of Waste/ byproducts; maximum incorporation of the materials used in the process into the final products (Atom Economy); prevention/ minimization of hazardous/ toxic products; designing safer chemicals – different basic approaches to do so; selection of appropriate auxiliary substances (solvents, separation agents), green solvents, solventless processes, immobilized solvents and ionic liquids; energy requirements for reactions - use of microwaves, ultrasonic energy; selection of starting materials; avoidance of unnecessary derivatization – careful use of blocking/protecting groups; use of catalytic reagents (wherever possible) in preference to stoichiometric reagents; designing of biodegradable products; prevention of chemical accidents; strengthening/ development of analytical techniques to prevent and minimize the generation of hazardous substances in chemical processes.

(24 Lectures)

Examples of Green Synthesis/ Reactions

1. Green Synthesis of the following compounds: adipic acid, catechol, BHT, methyl methacrylate, urethane, citral, ibuprofen, paracetamol, furfural.
 2. Microwave assisted reactions in water: Oxidation of toluene, alcohols.
- Microwave assisted reactions in organic solvents: Esterification, Fries rearrangement,

Diels-Alder Reaction.

Microwave assisted solid state reactions: Deacetylation, Deprotection. Saponification of esters, Alkylation of reactive methylene compounds, reductions, benzimidazoles.

3. Selective methylation of active methylene group using dimethylcarbonate; Solid-state polymerization of amorphous polymers using diphenylcarbonate; Use of “Clayan”, a nonmetallic oxidative reagent for various reactions; Free Radical Bromination; Role of Tellurium in organic syntheses; Biocatalysis in organic syntheses.

(24 Lectures)

Future Trends in Green Chemistry

Oxidation reagents and catalysts; Biomimetic, multifunctional reagents; Solventless reactions; Green chemistry in sustainable development.

(8 Lectures)

Recommended Books:

1. V.K. Ahluwalia & M.R. Kidwai: New Trends in Green Chemistry, Anamalaya Publishers (2005).
2. P.T. Anastas & J.K. Warner: Oxford Green Chemistry- Theory and Practical, University Press (1998).
3. A.S. Matlack: Introduction to Green Chemistry, Marcel Dekker (2001).
4. M.C. Cann & M.E. Connely: Real-World cases in Green Chemistry, American Chemical Society, Washington (2000).
5. M.A. Ryan & M. Tinnesand, Introduction to Green Chemistry, American Chemical Society, Washington (2002).

LAB: GREEN CHEMISTRY

60 Lectures

1. Safer starting materials

The Vitamin C clock reaction using Vitamin C tablets, tincture of iodine, hydrogen peroxide and liquid laundry starch.

- (i) Effect of concentration on clock reaction
- (ii) Effect of temperature on clock reaction.

2. Using renewable resources

Preparation of biodiesel from vegetable oil.

3. Avoiding waste

Principle of atom economy.

Use of molecular model kit to stimulate the reaction to investigate how the atom economy can illustrate Green Chemistry.

Preparation of propene by two methods can be studied

(I) Triethylamine ion + OH⁻ → propene + trimethylpropene + water

(II) 1-propanol $\xrightarrow{\text{H}_2\text{SO}_4/\Delta}$ propene + water

The other types of reactions, like addition, elimination, substitution and rearrangement should also be studied for the calculation of atom economy.

4. Use of enzymes as catalysts

Benzoin condensation using Thiamine Hydrochloride as a catalyst instead of cyanide

Alternative Green solvents

5. Diels Alder reaction in water

Reaction between furan and maleic acid in water and at room temperature rather than in benzene and reflux.

6. Extraction of D-limonene from orange peel using liquid CO₂ prepared from dry ice.

7. Mechanochemical solvent free synthesis of azomethines

8. Co-crystal controlled solid state synthesis (C₂S₃) of N-organophthalimide using phthalic anhydride and 3-aminobenzoic acid.

Alternative sources of energy

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

10. Photoreduction of benzophenone to benzopinacol in the presence of sunlight.

Recommended Books:

1. Anastas, P.T & Warner, J.C. *Green Chemistry: Theory and Practice*, Oxford University Press (1998).
 2. Kirchoff, M. & Ryan, M.A. *Greener approaches to undergraduate chemistry experiment*. American Chemical Society, Washington DC (2002).
 3. Ryan, M.A. *Introduction to Green Chemistry*, Tinnesand; (Ed), American Chemical Society, Washington DC (2002).
 4. Sharma, R.K.; Sidhwani, I.T. & Chaudhari, M.K. *Green Chemistry Experiment: A monograph*, I.K International Publishing House Pvt Ltd. New Delhi. Bangalore CISBN 978-93-81141-55-7 (2013).
 5. Cann, M.C. & Connelly, M. E. *Real world cases in Green Chemistry*, American Chemical Society (2008).
 6. Cann, M. C. & Thomas, P. *Real world cases in Green Chemistry*, American Chemical Society (2008).
 7. Pavia, D. L. Lampman, G. H. & Kriz, G.S. *W B Introduction to Organic Laboratory Techniques: A Microscale Approach*, 4th Ed., Brooks/Cole; 2007.
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CHE-RE-6026: INDUSTRIAL CHEMICALS AND ENVIRONMENT

(Credits: Theory-04, Lab -02)

Theory: 60 Lectures

Course Objectives: This course provides an introduction to the various industrial gases and inorganic chemicals, their manufacturing processes, applications, storage and the hazards of handling them. Contribution of these industrial chemicals towards air and water pollution and their effects on living organisms and the environment has also been covered. Students

are also expected to learn about metallurgy, energy generation industry and the pollution threat they pose. This course also discusses about management of the different kinds of wastes, their safe disposal and the importance of practicing green chemistry in chemical industry.

Learning Outcomes: After successful completion of the course, students would have learnt about the manufacture, applications and safe ways of storage and handling gaseous and inorganic industrial chemicals. Students will get to know about industrial metallurgy and the energy generation industry. Students will also learn about environmental pollution by various gaseous, liquid wastes and nuclear wastes and their effects on living beings. Finally, the students will learn about industrial waste management, their safe disposal and the importance of environment friendly “green chemistry” in chemical industry.

Industrial Gases and Inorganic Chemicals

Industrial Gases: Large scale production, uses, storage and hazards in handling of the following gases: oxygen, nitrogen, argon, neon, helium, hydrogen, acetylene, carbon monoxide, chlorine, fluorine, sulphur dioxide and phosgene.

Inorganic Chemicals: Manufacture, application, analysis and hazards in handling the following chemicals: hydrochloric acid, nitric acid, sulphuric acid, caustic soda, common salt, borax, bleaching powder, sodium thiosulphate, hydrogen peroxide, potash alum, chrome alum, potassium dichromate and potassium permanganate.

(10 Lectures)

Industrial Metallurgy

Preparation of metals (ferrous and nonferrous) and ultrapure metals for semiconductor technology.

(4 Lectures)

Environment and its segments

Ecosystems. Biogeochemical cycles of carbon, nitrogen and sulphur.

Air Pollution: Major regions of atmosphere. Chemical and photochemical reactions in atmosphere. Air pollutants: types, sources, particle size and chemical nature; Photochemical smog: its constituents and photochemistry. Environmental effects of ozone, Major sources of air pollution.

Pollution by SO₂, CO₂, CO, NO_x, H₂S and other foul smelling gases. Methods of estimation of CO, NO_x, SO_x and control procedures.

Effects of air pollution on living organisms and vegetation. Greenhouse effect and Global warming, Ozone depletion by oxides of nitrogen, chlorofluorocarbons and Halogens, removal of sulphur from coal. Control of particulates.

Water Pollution: Hydrological cycle, water resources, aquatic ecosystems, Sources and nature of water pollutants, Techniques for measuring water pollution, Impacts of water pollution on hydrological and ecosystems.

Water purification methods. Effluent treatment plants (primary, secondary and tertiary treatment). Industrial effluents from the following industries and their treatment: electroplating, textile, tannery, dairy, petroleum and petrochemicals, agro, fertilizer, etc. Sludge disposal.

Industrial waste management, incineration of waste. Water treatment and purification (reverse osmosis, electro dialysis, ion exchange). Water quality parameters for waste water, industrial water and domestic water.

(30 Lectures)

Energy & Environment

Sources of energy: Coal, petrol and natural gas. Nuclear Fusion / Fission, Solar energy, Hydrogen, geothermal, Tidal and Hydel, etc.

Nuclear Pollution: Disposal of nuclear waste, nuclear disaster and its management.

(10 Lectures)

Biocatalysis

Introduction to biocatalysis: Importance in “Green Chemistry” and Chemical Industry.

(6 Lectures)

Recommended Books:

1. E. Stocchi: *Industrial Chemistry*, Vol-I, Ellis Horwood Ltd. UK.
 2. R.M. Felder, R.W. Rousseau: *Elementary Principles of Chemical Processes*, Wiley Publishers, New Delhi.
 3. J. A. Kent: Riegel's *Handbook of Industrial Chemistry*, CBS Publishers, New Delhi.
 4. S. S. Dara: *A Textbook of Engineering Chemistry*, S. Chand & Company Ltd. New Delhi.
 5. K. De, *Environmental Chemistry*: New Age International Pvt., Ltd, New Delhi.
 6. S. M. Khopkar, *Environmental Pollution Analysis*: Wiley Eastern Ltd, New Delhi.
 7. S.E. Manahan, *Environmental Chemistry*, CRC Press (2005).
 8. G.T. Miller, *Environmental Science* 11th edition. Brooks/ Cole (2006).
 9. A. Mishra, *Environmental Studies*. Selective and Scientific Books, New Delhi (2005).
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LAB: INDUSTRIAL CHEMICALS & ENVIRONMENT

60 Lectures

1. Determination of dissolved oxygen in water.
2. Determination of Chemical Oxygen Demand (COD)
3. Determination of Biological Oxygen Demand (BOD)
4. Percentage of available chlorine in bleaching powder.
5. Measurement of chloride, sulphate and salinity of water samples by simple titration method (AgNO_3 and potassium chromate).
6. Estimation of total alkalinity of water samples (CO_3^{2-} , HCO_3^-) using double titration method.
7. Measurement of dissolved CO_2 .
8. Study of some of the common bio-indicators of pollution.
9. Estimation of SPM in air samples.
10. Preparation of borax/ boric acid.

Recommended Books:

1. E. Stocchi: *Industrial Chemistry*, Vol-I, Ellis Horwood Ltd. UK.
 2. R.M. Felder, R.W. Rousseau: *Elementary Principles of Chemical Processes*, Wiley Publishers, New Delhi.
 3. J. A. Kent: Riegel's *Handbook of Industrial Chemistry*, CBS Publishers, New Delhi.
 4. S. S. Dara: *A Textbook of Engineering Chemistry*, S. Chand & Company Ltd. New Delhi.
 5. K. De, *Environmental Chemistry*: New Age International Pvt., Ltd, New Delhi.
 6. S. M. Khopkar, *Environmental Pollution Analysis*: Wiley Eastern Ltd, New Delhi.
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CHE-RE-6036: INORGANIC MATERIALS OF INDUSTRIAL IMPORTANCE

(Credits: Theory-04, Lab -02)

Theory: 60 Lectures

Course Objectives: To learn the synthetic process, properties and the utility of the industrially important inorganic materials (such as silicates, ceramics, cements, fertilizers, paints, batteries, alloys and explosives).

To provide opportunity to learn some of the industrial process such as surface coating and catalysis in relevant to industry where heterogeneous catalysis dominates.

Experiments are aimed at helping learners acquire hands on experience in qualitative and quantitative analysis of the inorganic materials which are basically manufactured in chemical industries.

To learn some industrial techniques such as surface coating etc..

Learning Outcome: This course will establish the basic foundation of industrial inorganic chemistry among the students. This will be helpful for pursuing further studies of industrial chemistry in future. Experiments will help the Students to gather the experience of qualitative and quantitative chemical analysis. Students will be capable of doing analysis of the inorganic materials which are used in our daily life. They will have insight of the industrial processes.

Silicate Industries

Glass: Glassy state and its properties, classification (silicate and non-silicate glasses). Manufacture and processing of glass. Composition and properties of the following types of glasses: Soda lime glass, lead glass, armoured glass, safety glass, borosilicate glass, fluorosilicate, coloured glass, photosensitive glass.

Ceramics: Important clays and feldspar, ceramic, their types and manufacture. High technology ceramics and their applications, superconducting and semiconducting oxides,fullerenes carbon nanotubes and carbon fibre.

Cements: Classification of cement, ingredients and their role, Manufacture of cement and the setting process, quick setting cements.

(16 Lectures)

Fertilizers:

Different types of fertilizers. Manufacture of the following fertilizers: Urea, ammonium nitrate, calcium ammonium nitrate, ammonium phosphates; polyphosphate, superphosphate, compound and mixed fertilizers, potassium chloride, potassium sulphate.

(8 Lectures)

Surface Coatings:

Objectives of coatings surfaces, preliminary treatment of surface, classification of surface coatings. Paints and pigments-formulation, composition and related properties. Oil paint, Vehicle, modified oils, Pigments, toners and lakes pigments, Fillers, Thinners, Enamels, emulsifying agents. Special paints (Heat retardant, Fire retardant, Eco-friendly paint, Plastic paint), Dyes, Wax polishing, Water and Oil paints, additives, Metallic coatings (electrolytic and electroless), metal spraying and anodizing.

(10 Lectures)

Batteries:

Primary and secondary batteries, battery components and their role, Characteristics of battery. Working of following batteries: Pb acid, Li-Battery, Solid state electrolyte battery. Fuel cells, Solar cell and polymer cell.

(6 Lectures)

Alloys:

Classification of alloys, ferrous and non-ferrous alloys, Specific properties of elements in alloys. Manufacture of Steel (removal of silicon decarbonization, demanganization, desulphurization dephosphorisation) and surface treatment (argon treatment, heat treatment, nitriding, carburizing). Composition and properties of different types of steels.

(10 Lectures)

Catalysis:

General principles and properties of catalysts, homogenous catalysis (catalytic steps and examples) and heterogenous catalysis (catalytic steps and examples) and their industrial applications, Deactivation or regeneration of catalysts.

Phase transfer catalysts, application of zeolites as catalysts.

(6 Lectures)

Chemical explosives:

Origin of explosive properties in organic compounds, preparation and explosive properties of lead azide, PETN, cyclonite (RDX). Introduction to rocket propellants.

(4 Lectures)

Recommended Books:

1. E. Stocchi: *Industrial Chemistry*, Vol-I, Ellis Horwood Ltd. UK.
2. R. M. Felder, R. W. Rousseau: *Elementary Principles of Chemical Processes*, Wiley Publishers, New Delhi.
3. W. D. Kingery, H. K. Bowen, D. R. Uhlmann: *Introduction to Ceramics*, Wiley Publishers, New Delhi.
4. Karl Heinz Büchel, Hans-Heinrich Moretto Peter, Woditsch; *Industrial Inorganic Chemistry*, Wiley-VCH.
5. J. A. Kent: Riegel's *Handbook of Industrial Chemistry*, CBS Publishers, New Delhi.

6. P. C. Jain, M. Jain: *Engineering Chemistry*, Dhanpat Rai & Sons, Delhi.
 7. R. Gopalan, D. Venkappayya, S. Nagarajan: *Engineering Chemistry*, Vikas Publications, New Delhi.
 8. B. K. Sharma: *Engineering Chemistry*, Goel Publishing House, Meerut
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LAB: INORGANIC MATERIALS OF INDUSTRIAL IMPORTANCE

60 Lectures

1. Determination of free acidity in ammonium sulphate fertilizer.
2. Estimation of Calcium in Calcium ammonium nitrate fertilizer.
3. Estimation of phosphoric acid in superphosphate fertilizer.
4. Electroless metallic coatings on ceramic and plastic material.
5. Determination of composition of dolomite (by complexometric titration).
6. Analysis of (Cu, Ni); (Cu, Zn) in alloy or synthetic samples.
7. Analysis of Cement.
8. Preparation of pigment (zinc oxide).

Recommended Books:

1. E. Stocchi: *Industrial Chemistry*, Vol-I, Ellis Horwood Ltd. UK.
 2. R. M. Felder, R. W. Rousseau: *Elementary Principles of Chemical Processes*, Wiley Publishers, New Delhi.
 3. W. D. Kingery, H. K. Bowen, D. R. Uhlmann: *Introduction to Ceramics*, Wiley Publishers, New Delhi.
 4. J. A. Kent: Riegel's *Handbook of Industrial Chemistry*, CBS Publishers, New Delhi.
 5. P. C. Jain, M. Jain: *Engineering Chemistry*, Dhanpat Rai & Sons, Delhi.
 6. R. Gopalan, D. Venkappayya, S. Nagarajan: *Engineering Chemistry*, Vikas Publications, New Delhi.
 7. B. K. Sharma: *Engineering Chemistry*, Goel Publishing House, Meerut
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CHE-RE-6046: RESEARCH METHODOLOGY FOR CHEMISTRY

(Credits: Theory-05, Tutorials-01)

Theory: 75 Lectures

Course Objectives:

This course is introduced to impart knowledge about the basic concepts of research and to provide a road map for conducting research

Students are expected to identify, explain and apply basic concepts of research; acquire information, recognize various issues related to research and to learn instrumental methods required for research in chemistry.

Learning Outcome:

After completing this course, students should be able to construct a rational research proposal to generate fruitful output in terms of publications and patents in the field of chemical sciences.

Literature Survey:

Print: Sources of information: Primary, secondary, tertiary sources; Journals: Journal

abbreviations, abstracts, current titles, reviews, monographs, dictionaries, text-books, current contents, Introduction to Chemical Abstracts and Beilstein, Subject Index, Substance Index, Author Index, Formula Index, and other Indices with examples.

Digital: Web resources, E-journals, Journal access, TOC alerts, Hot articles, Citation index, Impact factor, H-index, E-consortium, UGC infonet, E-books, Internet discussion groups and

communities, Blogs, Preprint servers, Search engines, Scirus, Google Scholar, ChemIndustry, Wiki- Databases, ChemSpider, Science Direct, SciFinder, Scopus.

Information Technology and Library Resources: The Internet and World Wide Web. Internet resources for chemistry. Finding and citing published information.

(20 Lectures)

Methods of Scientific Research and Writing Scientific Papers:

Reporting practical and project work. Writing literature surveys and reviews. Organizing a poster display. Giving an oral presentation.

Writing scientific papers – justification for scientific contributions, bibliography, description of methods, conclusions, the need for illustration, style, publications of scientific work. Writing ethics. Avoiding plagiarism.

(20 Lectures)

Chemical Safety and Ethical Handling of Chemicals:

Safe working procedure and protective environment, protective apparel, emergency procedure and first aid, laboratory ventilation. Safe storage and use of hazardous chemicals, procedure for working with substances that pose hazards, flammable or explosive hazards, procedures for working with gases at pressures above or below atmospheric – safe storage and disposal of waste chemicals, recovery, recycling and reuse of laboratory chemicals, procedure for laboratory disposal of explosives, identification, verification and segregation of laboratory waste, disposal of chemicals in the sanitary sewer system, incineration and transportation of hazardous chemicals.

(12 Lectures)

Data Analysis

The Investigative Approach: Making and Recording Measurements. SI Units and their use. Scientific method and design of experiments.

Analysis and Presentation of Data: Descriptive statistics. Choosing and using statistical tests. Chemometrics. Analysis of variance (ANOVA), Correlation and regression, Curve fitting, fitting of linear equations, simple linear cases, weighted linear case, analysis of residuals, General polynomial fitting, linearizing transformations, exponential function fit, r and its abuse. Basic aspects of multiple linear regression analysis.

(13 Lectures)

Electronics

Basic fundamentals of electronic circuits and their components used in circuits of common instruments like spectrophotometers, typical circuits involving operational amplifiers for electrochemical instruments. Elementary aspects of digital electronics.

(10 Lectures)

Recommended Books

1. Dean, J. R., Jones, A. M., Holmes, D., Reed, R., Weyers, J. & Jones, A. (2011) *Practical skills in chemistry*. 2nd Ed. Prentice-Hall, Harlow.
 2. Hibbert, D. B. & Gooding, J. J. (2006) *Data analysis for chemistry*. Oxford University Press.
 3. Topping, J. (1984) *Errors of observation and their treatment*. Fourth Ed., Chapman Hall, London.
 4. Harris, D. C. *Quantitative chemical analysis*. 6th Ed., Freeman (2007) Chapters 3-5.
 5. Levie, R. de, *How to use Excel in analytical chemistry and in general scientific data analysis*. Cambridge Univ. Press (2001) 487 pages.
 6. Chemical safety matters – IUPAC – IPCS, Cambridge University Press, 1992.
 7. OSU safety manual 1.01.
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CHEM-HE-6056: Dissertation

Student will complete a project work and then prepare a report on that.

Skill Enhancement Course (SEC)

AAA-SE-3014: ENGLISH

(Credits: 04)

60 Lectures

Syllabus will be available at GU website

CHE-SE-3024: IT SKILLS FOR CHEMISTS

(Credits: 04) 60 Lectures

Course Objective: The objectives of the proposed course are:

- 1) *To provide the basic knowledge of mathematics which are needed to pursue chemistry as major subject.*
- 2) *To provide the necessary training for the basic programming knowledge.*
- 3) *The course provides information technology literacy and basic skills training for learners with limited experience.*
- 4) *To familiarize with the Introductory writing activities and Handling numeric data.*

Learning Outcome: *Course learning outcomes focus on skill development related to basic computer operations and information technology. After completing the course the incumbent is able to use the computer for basic purposes of preparing his personnel/business letters, viewing information on Internet (the web), sending mails, using internet banking services etc. After opting this course the students are expected to accumulate the skills in writing activities and Handling numeric data.*

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. BASIC keywords and commands. Logical and relative operators. Strings and graphics. Compiled versus interpreted languages. Errors (Syntax and Logical), 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/Latex.

Handling numeric data: Spreadsheet software (Excel), 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, 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, pK_a 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. Statistical significance testing: The t test. The F test.

Presentation: Presentation graphics

Recommended Books:

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

CHE-SE-3034: BASIC ANALYTICAL CHEMISTRY
(Credits: 04) 60 Lectures

Course Objective: To familiarize students with different micro and semimicro analytical techniques and help develop the ability to use modern instrumental methods for chemical analysis of food, soil, air and water.

Learning Outcome: Upon completion of this course, students shall be able to explain the basic principles of chemical analysis, design/implement microscale and semimicro experiments, record, interpret and analyze data following scientific methodology.

Introduction: Introduction to Analytical Chemistry and its interdisciplinary nature. Concept of sampling. Importance of accuracy, precision and sources of error in analytical measurements. Presentation 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

- Determination of pH of soil samples.
- 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.

- Determination of pH, acidity and alkalinity of a water sample.
- Determination of dissolved oxygen (DO) of a water sample.

Analysis of food products: Nutritional value of foods, idea about food processing and food preservations and adulteration.

- Identification of adulterants in some common food items like coffee powder, asafoetida, chilli powder, turmeric powder, coriander powder and pulses, etc.
- Analysis of preservatives and colouring matter.

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

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

Analysis of cosmetics: Major and minor constituents and their function

- Analysis of deodorants and antiperspirants, Al, Zn, boric acid, chloride, sulphate.
- Determination of constituents of talcum powder: Magnesium oxide, Calcium oxide, Zinc oxide and Calcium carbonate by complexometric titration.

Suggested Applications (Any one):

- To study the use of phenolphthalein in trap cases.
- To analyze arson accelerants.
- 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 Drink.

Recommended Books:

1. Willard, H. H. *Instrumental Methods of Analysis*, CBS Publishers.
2. Skoog & Lerry. *Instrumental Methods of Analysis*, Saunders College Publications, New York.
3. Skoog, D.A.; West, D.M. & Holler, F.J. *Fundamentals of Analytical Chemistry 6th Ed.*, Saunders College Publishing, Fort Worth (1992).
4. Harris, D. C. *Quantitative Chemical Analysis*, W. H. Freeman.
5. Dean, J. A. *Analytical Chemistry Notebook*, McGraw Hill.
6. Day, R. A. & Underwood, A. L. *Quantitative Analysis*, Prentice Hall of India.
7. Freifelder, D. *Physical Biochemistry 2nd Ed.*, W.H. Freeman and Co., N.Y. USA(1982).
8. Cooper, T.G. *The Tools of Biochemistry*, John Wiley and Sons, N.Y. USA. 16(1977).
9. Vogel, A. I. *Vogel's Qualitative Inorganic Analysis 7th Ed.*, Prentice Hall.
10. Vogel, A. I. *Vogel's Quantitative Chemical Analysis 6th Ed.*, Prentice Hall.
11. Robinson, J.W. *Undergraduate Instrumental Analysis 5th Ed.*, Marcel Dekker, Inc., New York (1995).

CHE-SE-4014: ANALYTICAL CLINICAL BIOCHEMISTRY

(Credits: 04) 60 Lectures

Course objective: This course is intended to apprise students with various clinically relevant biomolecules, their structures and physiological roles. Students are also expected to learn the basics of analysis of pathological samples (blood and urine).

Learning outcome: Students will be able to identify various molecules relevant to a particular pathological condition and their estimation protocols.

Basic understanding of the structures, properties and functions of carbohydrates, lipids and proteins:

Review of concepts studied in the core course.

Carbohydrates: Biological importance of carbohydrates, metabolism, cellular currency of energy (ATP), glycolysis, alcoholic and lactic acid fermentations, Krebs cycle, Isolation and characterization of polysachharides.

Proteins: Classification, biological importance, primary and secondary, tertiary and quaternary structures of proteins: α -helix and β -pleated sheets, isolation, characterization, denaturation of proteins.

Enzymes: Nomenclature, characteristics, classification, active site, mechanism of enzyme action, stereospecificity of enzymes, effect of pH, temperature on enzyme activity, , enzyme inhibitors, coenzymes and cofactors introduction to biocatalysis: importance in “Green Chemistry” and chemical industry.

Lipids: Classification, biological importance of triglycerides and phosphoglycerides and cholesterol, lipid membrane, liposomes and their biological functions and underlying applications.

Lipoproteins.

Properties, functions and biochemical functions of steroid hormones.

Biochemistry of peptide hormones.

Structure of DNA (Watson-Crick model) and RNA, genetic code, biological roles of DNA and RNA: replication, transcription and translation, introduction to gene therapy.

Biochemistry of disease: A diagnostic approach by blood/ urine analysis:

Blood: Composition and functions of blood, blood coagulation, blood collection and preservation of samples, anemia, regulation, estimation and interpretation of data for blood sugar, urea, creatinine, cholesterol and bilirubin.

Urine: Collection and preservation of samples, formation of urine, composition and estimation of constituents of normal and pathological urine.

Practicals:

Identification and estimation of the following:

1. Carbohydrates - qualitative and quantitative analysis.
2. Lipids - qualitative and quantitative analysis.
3. Determination of the iodine number of oil.
4. Determination of the saponification number of oil.
5. Detection of cholesterol using Liebermann- Burchard reaction.
6. Isolation of protein.
7. Determination of concentration of protein by the Biuret reaction.
8. Determination of nucleic acid concentration.
9. Separation of nucleic acids.

Recommended Books:

1. David L. Nelson and Michael M. Cox: Lehninger Principles of Biochemistry
2. T.G. Cooper: Tool of Biochemistry.
3. Keith Wilson and John Walker: Practical Biochemistry.
4. Alan H Gowenlock: Varley’s Practical Clinical Biochemistry.
5. Thomas M. Devlin: Textbook of Biochemistry.
6. Jeremy M. Berg, John L Tymoczko, Lubert Stryer: Biochemistry.
7. G. P. Talwar and M Srivastava: Textbook of Biochemistry and Human Biology.
8. O. Mikes, R.A. Chalmers: Laboratory Handbook of Chromatographic Methods.

CHE-SE-4024: GREEN METHODS IN CHEMISTRY

(Credits: 04) 60 Lectures

Course Objectives: This course introduces students to the utilization of green chemistry from industrial perspective and provides exposure to methods by which environmental problems are evaluated and designing of sustainable solutions.

Learning Outcome: Students shall be able to describe and evaluate chemical products and processes from environmental perspective, define and propose sustainable solutions and critically assess the methods for waste reduction and recycling.

Tools of Green chemistry, Twelve principles of Green Chemistry, with examples.

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

- 1 A green synthesis of ibuprofen which creates less waste and fewer byproducts (Atom economy).
- 2 Surfactants for Carbon Dioxide – replacing smog producing and ozone depleting solvents with CO₂ for precision cleaning and dry cleaning of garments.
- 3 Environmentally safe antifoulant.
- 4 CO₂ as an environmentally friendly blowing agent for the polystyrene foam sheet packaging market.
- 5 Using a catalyst to improve the delignifying (bleaching) activity of hydrogen peroxide.
- 6 A new generation of environmentally advanced preservative: getting the chromium and arsenic out of pressure treated wood.
7. Rightfit pigment: synthetic azopigments to replace toxic organic and inorganic pigments.
- 8 Development of a fully recyclable carpet: cradle to cradle carpeting.

Recommended Books:

1. Manahan S.E. (2005) Environmental Chemistry, CRC Press
 2. Miller, G.T. (2006) Environmental Science 11th edition. Brooks/Cole
 3. Mishra, A. (2005) Environmental Studies. Selective and Scientific Books, New
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CHE-SE-4034: PHARMACEUTICAL CHEMISTRY

(Credits: 04) 60 Lectures

Course Objective: This primary objective of this course is to introduce students to the fundamentals of drug design and development process, drugs for various diseases available in market, their mode of action and side effects. Students are expected to learn the biosynthetic procedures of various bio-relevant small molecules.

Learning Outcome: Students will be able to appreciate the drug development process, identify various small molecules used for treatments different ailments and other physiological processes.

Drugs & Pharmaceuticals:

Drug discovery, design and development; basic retrosynthetic approach, synthesis of the representative drugs of the following classes: analgesics, antipyretic, anti-inflammatory (aspirin, paracetamol, ibuprofen), antibiotics (chloramphenicol), antibacterial and antifungal (sulphonamides, sulphamethoxazol, sulphacetamide, trimethoprim), antiviral (acyclovir), drugs effecting central nervous system (phenobarbital, diazepam), cardiovascular (glyceryl trinitrate), antilaprosy (dapson), HIV-AIDS related drugs (AZT- Zidovudine).

Fermentation:

Aerobic and anaerobic fermentation, production of (i) ethanol 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).

Recommended Books:

1. Graham L. Patrick: *An Introduction to Medicinal Chemistry*, Oxford University Press, UK.
 2. Gareth Thomas: *Fundamentals of Medicinal Chemistry*, Wiley.
 3. Hakishan, V.K. Kapoor: *Medicinal and Pharmaceutical Chemistry*, Vallabh Prakashan, Pitampura, New Delhi.
 4. William O. Foye, Thomas L., Lemke, David A. William: *Principles of Medicinal Chemistry*, B.I. Waverly Pvt. Ltd. New Delhi.
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CHE-SE-5014: CHEMICAL TECHNOLOGY & SOCIETY

(Credits: 04) 60 Lectures

Course Objective: The objective of the course is to enable students to have a firsthand understanding of different types of equipments needed in chemical technology and offer them concepts regarding some important parameters. The syllabus also emphasizes the dynamic nature of the relations between society on one hand and technological achievement from chemical industries on the other hand. In other words, it tries to explore societal and technological issues from a chemical perspective.

Learning Outcome: Students shall be familiarized with processes and terminologies in chemical industry, like mass balance, energy balance etc... Learners will be able to use chemical and scientific literacy as a means to better understand the topics related to the society.

Chemical Technology

Different types of equipments needed in chemical technology, including reactors, distillation columns, extruders, pumps, mills, emulgators. Scaling up operations in chemical industry. Introduction to clean technology.

Concept of relative humidity, molal humidity, dew point, partial saturation.

Material Balance: Recycle, bypass in batch, stage wise and continuous operations in systems with and without chemical reactions.

Energy balance: Energy balance of systems with and without chemical reactions.

Society

Social issues related to soil, air and water pollution.

Energy crisis of modern society and search for alternatives such as energy from natural sources (i.e. solar and renewable forms), and from nuclear fission, biofuel etc.

Pros and cons of use of materials like plastics and polymers and their natural analogues,

Genetic engineering and the manufacture of drugs (proteins and nucleic acids, and molecular reactivity and interconversions)

Recommended Book:

1. John W. Hill, Terry W. McCreary & Doris K. Kolb, *Chemistry for changing times* 13th Ed.
2. E.J. Hackett, O. Amsterdamska, M. Lynch and J. Wajcman (eds.), *The Handbook of Science and Technology Studies*, The MIT Press, 2008.
3. D. MacKenzie and J. Wajcman (eds.), *The Social Shaping of Technology*, The Open University Press, 1999.

CHE-SE-5024: CHEMOINFORMATICS

(Credits: 04) 60 Lectures

Learning Objectives: *The primary objective of this course is to familiarize the students with the use of various computer softwares and information technology. The students are expected to learn different chemical search engines and utilize them for molecular modelling and structure elucidation with a final goal to compute NMR, IR, mass and other spectra that can be later compared with the experimental data. The course also provides sufficient information and hands on exercises on the use of cheminformatics, with a special emphasis on its application in modern drug discovery.*

Learning Outcomes: *On the successful completion of the course, the students should be able to explain, interpret and critically examine the utility of computers and software tools to solving chemistry related problems. Recognize, apply, compare and predict chemical structures, properties, and reactivity and; solve chemistry related problems.*

Employ critical thinking and scientific reasoning to design and safely implement laboratory experiments and keep the records of the same.

Compile, interpret and analyze the qualitative/quantitative data and communicate the same in a scientific literature

Introduction to Chemoinformatics: History and evolution of chemoinformatics, Use of chemoinformatics, Prospects of chemoinformatics, Molecular Modelling and Structure elucidation.

Representation of molecules and chemical reactions: Nomenclature, Different types of notations, SMILES coding, Matrix representations, Structure of Molfiles and Sdfiles, Libraries and toolkits, Different electronic effects, Reaction classification.

Searching chemical structures: Full structure search, sub-structure search, basic ideas, similarity search, three dimensional search methods, basics of computation of physical and chemical data and structure descriptors, data visualization.

Applications: Prediction of Properties of Compounds; Linear Free Energy Relations; Quantitative Structure-Property Relations; Descriptor Analysis; Model Building; Modeling Toxicity; Structure-Spectra correlations; Prediction of NMR, IR and Mass spectra; Computer Assisted Structure elucidations; Computer Assisted Synthesis Design, Introduction to drug design; Target Identification and Validation; Lead Finding and Optimization; Analysis of HTS data; Virtual Screening; Design of Combinatorial Libraries; Ligand-Based and Structure Based Drug design; Application of Chemoinformatics in Drug Design.

Hands-on Exercises

Recommended Books:

1. Andrew R. Leach & Valerie, J. Gillet (2007) *An introduction to Chemoinformatics*. Springer: The Netherlands.
2. Gasteiger, J. & Engel, T. (2003) *Chemoinformatics: A text-book*. Wiley-VCH.
3. Gupta, S. P. (2011) *QSAR & Molecular Modeling*. Anamaya Pub.: New Delhi.

CHE-SE-5034: BUSINESS SKILLS FOR CHEMISTS (Credits: 04) 60 Lectures

Course Objective: To familiarize students with important concepts of business operations and intellectual rights as applied to chemical industry.

Learning outcome: students shall be able to explain and/or analyze the important steps of business operations, finance and intellectual property as applied to chemical industry.

Chemistry in Industry

Current challenges and opportunities for the chemistry-using industries, role of chemistry in India and global economies.

Basics of Business and Management

Key business concepts: Business plans, market need, project management and routes to market.

Management Functions and skills, principles of motivation, forms of business organization including partnerships and companies.

Marketing Skills

Understanding basics of marketing and marketing mix strategies with cases.

Human Resource Management (HRM) Skills

Managerial HRM functions viz. recruitment, training and development and compensation.

Financial Management Skills

An overview of financial and cost accounting with cases, managerial finance functions.

Intellectual Property Rights

Concept of intellectual property rights, patents.

Recommended books

1. <http://www.rsc.org/learn-chemistry/resources/business-skills-for-chemists/OnlineCourse/>
 2. Philip Kotler, Keven Lane Keller Marketing Management 15th Ed., Pearson Education; Fifteenth edition (10 August 2017)
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CHE-SE-5044: INTELLECTUAL PROPERTY RIGHTS

(Credits: 04) 60 Lectures

Course Objective: In this era of liberalization and globalization, the perception about science and its practices has undergone dramatic change. The importance of protecting the scientific discoveries, with commercial potential or the intellectual property rights is being discussed at all levels – statutory, administrative, and judicial. With India ratifying the WTO agreement, it has become obligatory on its part to follow a minimum acceptable standard for protection and enforcement of intellectual property rights. The purpose of this course is to apprise the students about the multifaceted dimensions of this issue.

Learning Outcome: After completing this course, students will have in-depth understanding about the importance and types of IPR. This course will also provide the clarity on the legal and economic aspects of the IP system.

Introduction to Intellectual Property:

Historical Perspective, Different Types of IP, Importance of protecting IP.

Copyrights

Introduction, How to obtain, Differences from Patents.

Trade Marks

Introduction, How to obtain, Different types of marks – Collective marks, certification marks, service marks, Trade names, etc.
Differences from Designs.

Patents

Historical Perspective, Basic and associated right, WIPO, PCT system, Traditional Knowledge, Patents and Healthcare – balancing promoting innovation with public health, Software patents and their importance for India.

Geographical Indications

Definition, rules for registration, prevention of illegal exploitation, importance to India.

Industrial Designs

Definition, How to obtain, features, International design registration.

Layout design of integrated circuits

Circuit Boards, Integrated Chips, Importance for electronic industry.

Trade Secrets

Introduction and Historical Perspectives, Scope of Protection, Risks involved and legal aspects of Trade Secret Protection.

Different International agreements

(a) World Trade Organization (WTO):

- (i) General Agreement on Tariffs & Trade (GATT), Trade Related Intellectual Property Rights (TRIPS) agreement
- (ii) General Agreement on Trade related Services (GATS)
- (iii) Madrid Protocol
- (iv) Berne Convention
- (v) Budapest Treaty

(b) Paris Convention

WIPO and TRIPS, IPR and Plant Breeders Rights, IPR and Biodiversity

IP Infringement issue and enforcement – Role of Judiciary, Role of law enforcement agencies – Police, Customs etc. Economic Value of Intellectual Property – Intangible assets and their valuation, Intellectual Property in the Indian Context – Various laws in India Licensing and technology transfer.

Recommended Books:

1. N.K. Acharya: *Textbook on intellectual property rights*, Asia Law House (2001).
2. Manjula Guru & M.B. Rao, *Understanding Trips: Managing Knowledge in Developing Countries*, Sage Publications (2003).
3. P. Ganguli, *Intellectual Property Rights: Unleashing the Knowledge Economy*, Tata McGraw-Hill (2001).
4. Arthur Raphael Miller, Micheal H.Davis; *Intellectual Property: Patents, Trademarks*

- and Copyright in a Nutshell*, West Group Publishers (2000).
- Jayashree Watal, *Intellectual property rights in the WTO and developing countries*, Oxford University Press, Oxford.
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CHE-SE-6014: CHEMISTRY OF COSMETICS & PERFUMES

(Credits: 04) 60 Lectures

Course Objective: This course intends to apprise students about the chemical knowledge related to some of the commonly used cosmetics. Laboratory experiments for preparation of talcum powder, shampoo etc. are included to give hands on experience.

Learning Outcome: Students will learn about the preparation and chemistry involved with the production different cosmetic. This may encourage students to take up entry level jobs at cosmetics industry or venture into commercial production of cosmetics as an entrepreneur.

A general study including preparation and uses of the following: Hair dye, hair spray, shampoo, suntan lotions, face powder, lipsticks, talcum powder, nail enamel, creams (cold,

vanishing and shaving creams), antiperspirants and artificial flavours. Essential oils and their importance in cosmetic industries with reference to Eugenol, Geraniol, sandalwood oil, eucalyptus, rose oil, 2-phenyl ethyl alcohol, Jasmone, Civetone, Muscone.

Practicals

- Preparation of talcum powder.
- Preparation of shampoo.
- Preparation of enamels.
- Preparation of hair remover.
- Preparation of face cream.
- Preparation of nail polish and nail polish remover.

Recommended Books:

- E. Stocchi: *Industrial Chemistry*, Vol -I, Ellis Horwood Ltd. UK.
 - P.C. Jain, M. Jain: *Engineering Chemistry*, Dhanpat Rai & Sons, Delhi.
 - B.K. Sharma: *Industrial Chemistry*, Goel Publishing House, Meerut.
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CHE-SE-6024: PESTICIDE CHEMISTRY

(Credits: 04) 60 Lectures

Course Objective: This is a brief and introductory course on pesticides, through which the students will be introduced to various classes of pesticides, their synthesis, applications and possible hazards of their uses.

Learning Outcome: Students will be able to explain or describe and critically examine different types of pesticides, their activity/toxicity and their applications and the need for the search of an alternative based on natural products.

Definition of pesticides, general introduction to pesticides (natural and synthetic), benefits and adverse effects of pesticides. Classification, mode of action, toxicity and methods of pesticides residue analysis. Synthesis and technical manufacture and uses of representative pesticides in the following classes: Organochlorines (DDT, Gammexene); organophosphate (Malathion, Parathion); Carbamates (Carbofuran and carbaryl); Quinones (Chloranil), Anilides (Alachlor and Butachlor)

Practicals:

1. To calculate acidity/alkalinity in given sample of pesticides formulations as per BIS specifications.
2. Preparation of simple organophosphates, phosphonates and thiophosphates.

Recommended Book:

1. R. Cremlyn: Pesticides, Preparation and Mode of Action, John Wiley & Sons, New York, 1978
2. RPBateman, Pesticide Applications, AAB Press, 2004
3. Principles of Pesticide chemistry: S K Handa, Ed. by Agrobios (India), 2008
4. Pesticide Science & Biotechnology: R Greenhalgh and T R Robers, IUPAC, Blackwell Scientific Publications, 1987
5. The Chemical Process Industries: D N Shreve
6. Pesticide Chemistry : G Matolesy, M. Nadasy, V. Andriska, Elsevier Sc. Publisher, USA, 1988

CHE-SE-6034: FUEL CHEMISTRY
(Credits: 04) 60 Lectures

Course Objectives: This course discusses about the chemistry of various sources of energy. Students are expected to learn about the composition of coal and petroleum products, their extraction, purification methods and usage. A section also covers classification and applications of natural and synthetic lubricants. Students will also learn about the determination and significance of various industrially relevant physical parameters for different fuels and lubricants.

Learning Outcomes: At the end of this course students will learn about the classes of renewable and non-renewable energy sources. Students will learn about the composition of coal and crude petroleum, their classification, isolation of coal and petroleum products and

their usage in various industries. They will also learn to determine industrially significant physical parameters for fuels and lubricants.

Fuel Chemistry

Review of energy sources (renewable and non-renewable). Classification of fuels and their calorific value.

Coal: Uses of coal (fuel and nonfuel) in various industries, its composition, carbonization of coal. Coal gas, producer gas and water gas—composition and uses. Fractionation of coal tar, uses of coal tar bases chemicals, requisites of a good metallurgical coke, Coal gasification (Hydro gasification and Catalytic gasification), Coal liquefaction and Solvent Refining.

Petroleum and Petrochemical Industry: Composition of crude petroleum, Refining and different types of petroleum products and their applications.

Fractional Distillation (Principle and process), Cracking (Thermal and catalytic cracking), Reforming Petroleum and non-petroleum fuels (LPG, CNG, LNG, bio-gas, fuels derived from biomass), fuel from waste, synthetic fuels (gaseous and liquids), clean fuels. Petrochemicals: Vinyl acetate, Propylene oxide, Isoprene, Butadiene, Toluene and its derivatives Xylene.

Lubricants: Classification of lubricants, lubricating oils (conducting and non-conducting) Solid and semisolid lubricants, synthetic lubricants.

Properties of lubricants (viscosity index, cloud point, pour point) and their determination.

Recommended Books:

1. E. Stocchi: *Industrial Chemistry*, Vol -I, Ellis Horwood Ltd. UK.
 2. P.C. Jain, M. Jain: *Engineering Chemistry*, Dhanpat Rai & Sons, Delhi.
 3. B.K. Sharma: *Industrial Chemistry*, Goel Publishing House, Meerut.
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