

THIRD YEAR

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THIRD YEAR**CH 301: SURFACE CHEMISTRY, COLLOIDS AND PHASE EQUILIBRIA 3 CREDITS**

Learning Objectives: This course content will help the learners to

- learn about the characterization techniques of solid surfaces.
- study the effect of temperature on adsorption and adsorption isotherm.
- acquire knowledge on self-assembled monolayer and multilayers formed on the air-water interface and on solid substrate.
- get idea about colloidal particles and emulsions, their properties and applications.
- learn different phase of a species and different theories related to phase equilibria.

Course Contents

1. **Surface Chemistry:** Solid surfaces and their characterization, surface active agents, surface tension, adsorption on solid surfaces, techniques for measurement of adsorption on solids from the gas phase and solutions, adsorption isotherms: Langmuir, Freundlich and BET, surface free energy, wetting, contact angle, surface forces, enthalpy of adsorption, role of adsorption in heterogeneous catalysis, applications of surface science in petroleum recovery, coating and painting, food, pharmaceutical and cosmetic industry.
2. **Adsorption on the Surface of Liquid:** Gibb's adsorption equation, determination of surface excess concentrations, electrocapillary phenomenon, surface films, surface pressure, determination of the cross sectional area of surface active molecules by surface tension measurements, Langmuir trough, Langmuir films, Langmuir-Blodgett films, preparation & characterization, nanofabrication with self-assembled monolayers, adsorption of polymer, stability and flocculation of colloids using polymer.
3. **The Colloidal State of Matter:** Classification, preparations, purifications and physical properties of colloids, structure and stability of colloids, the electrical double layer, zeta potential, flocculation, coagulation and Hardy-Schulze law, dispersion systems: sedimentation, rheology, electrokinetic phenomena, colloidal electrolytes and their uses. micelles and biological membranes, emulsions: preparation, properties, stability and uses of emulsions, microemulsions, applications of colloidal science in petroleum recovery, coating and painting, food, pharmaceutical and cosmetic industry.
4. **Phase Equilibria:** Phase rule and its application in one component system like water, sulfur, Duhem-Margules equation, completely and partially miscible liquid pairs, solid-liquid systems comprising two components, efflorescence and deliquescence, vapor pressure of saturated solutions, solid-solid binary systems with reference to alloys, cooling curves, systems

without compound formation, congruent and incongruent melting points, introductory ideas about ternary systems and triangular phase diagram.

Learning Outcomes: Upon completion of this course, the student should be able to

- explain different surface phenomena.
- prepare langmuir films at the air-water interface and Langmuir-Blodgett films on different types of solid surfaces.
- realize the micelles, reverse micelles and Tyndal effect of colloidal particles and prepare emulsions.
- explain the phase diagram of one/two component system.

Books Recommended

1. Colloidal Science, A. E. Alexender and P. Johnson.
2. Physical Chemistry, P. Atkins and J. de Paula, Oxford.
3. Colloidal Chemistry, B. Jirgenson and M. E. Straumains.
4. Text Book of Colloidal Chemistry, A. B. Weiser.
5. Phase Rule, A. Findlay (revised by Campbell).
6. Physical Chemistry of Surface, A.W. Advenson and A.P. Gast

CH 302: CHEMICAL KINETICS AND PHOTOCHEMISTRY

3 CREDITS

Learning Objectives: This course content will help the learners to

- acquire knowledge on the kinetics of elementary and composite reactions.
- learn about the techniques to measure reaction rates.
- study the theories of reaction rates.
- understand fundamentals of photochemical reactions and catalysis.
- distinguish between photochemistry and radiation chemistry.

Course Contents

1. **Chemical Kinetics:** Review of elementary concepts: order, molecularity and rate constant, integration of rate equations for model reaction systems: zero, first and 2nd order reactions, parallel, consecutive, successive and opposing reactions: methods for determination of order and rate constants, complex reactions, steady state approximation, kinetics of polymerization reactions, chain reactions, explosions.
2. **Techniques and Methods for Measuring Rates of Reactions:** Conventional chemical methods: conductance methods, polarimetry, spectrophotometry; methods based on gas pressure and volume measurements, techniques for measuring rates of fast reactions: production

and measurement of free radicals, flash photolysis, flow methods, relaxation techniques, relative methods.

3. **Temperature Dependence of Reaction Rates and Theories:** The Arrhenius equation, bimolecular reactions: collision theory-its success and failures, transition state theory: elementary treatment, Eyring equation, thermodynamic formulation, reaction enthalpy and enthalpy diagrams.
4. **Reactions in Solution:** Diffusion and activation controlled reactions, theories of reaction rate in solutions, effect of dielectric constant and ionic strength on rates of reactions in solution.
5. **Theories of Unimolecular Reactions:** Unimolecular reactions: Lindemann theory, Hinshelwood treatment.
6. **Kinetics and Reaction Mechanism:** Principle of steady state approximation, iodination of acetone, decomposition of nitrogen pentoxide, decomposition of ethane and acetaldehyde, hydrogen-chlorine, and hydrogen bromine reaction, hydrogenation of ethylene.
7. **Catalysis:** Homogeneous and heterogeneous catalysis, acid-base catalysis, Hinshelwood and Rideal mechanism, enzyme catalysis: Michael-Menten equation, autocatalysis, oscillatory reactions.
8. **Photochemistry and Photochemical Reaction:** Laws of photochemistry, quantum yield and its significance, light source, actinometer and its working principle, fates of photoexcited species, photodissociation, photoionization, some typical photochemical reactions, photosensitization and photocatalysis, mechanism of photocatalytic reactions, formation and depletion of ozone in the stratosphere, ozone hole.
9. **Radiation chemistry:** Types of radiation, difference between photochemistry and radiation chemistry, G-value and its significance.

Learning Outcomes: Upon completion of this course, the student should be able to

- determine the reaction rate for thermodynamically controlled reaction as well as for fast reaction.
- understand different theories of reaction rates, their limitations and their modifications.
- realize the mechanism of a catalyzed and non-catalyzed reaction.
- explain the photochemical laws, primary and secondary photochemical processes, determine quantum yield and interpret the data, describe photochemical chain and non-chain reactions.

Books Recommended

1. Reaction Kinetics, M. J. Pilling and P. W. Seakins, Oxford Science Publications.

2. Physical Chemistry, P. Atkins and J. de Paula, Oxford.
3. Kinetics of Chemical Change, C.N. Hinshelwood.
4. Chemical Kinetics, K.J. Laidler.
5. Chemical Kinetics and Dynamics by J. I. Steinfield, J. F. Francisco and W. L. Hase. Prentice Hall, New Jersey.
6. Chemical Kinetics, Kenneth A. Connors.
7. Introduction to Molecular Photochemistry, C. H. J. Wells.
8. Principles and Applications of Photochemistry, R. P. Wayne, Oxford. (1988).
9. Fundamentals of Photochemistry, K.K Rohatgi and Mukhargi.

CHL 303: PHYSICAL CHEMISTRY LABORATORY-II**2 CREDITS**

Learning Objectives: This course content will help the learners to

- impart skill on various experimental techniques.
- learn collecting experimental data.
- organize and interpret collected experimental data.

Course Contents

1. To determine the molar mass of a volatile substance by Victor Mayer's method.
2. To determine the equilibrium constant for the reaction $KI + I_2 \rightleftharpoons KI_3$
3. To determine the heat of neutralisation of a strong acid and a strong base.
4. To determine the heat of solution of a substance from solubility measurement.
5. To determine the velocity constant for the hydrolysis of an ester, catalysed by hydrogen ions (Titrimetric method).
6. To determine (a) the phase diagram for the phenol-water system and to find out the critical solution temperature and (b) to investigate the effect of added impurities on CST.
7. To determine the formula of the silverammine complex.
8. To determine the molar mass of a given liquid by steam distillation method.
9. To determine the solubility product of $Ca(OH)_2$ in H_2O and to study the effect of added $CaCl_2$ on the solubility of $Ca(OH)_2$
10. To verify of the Hess's law of constant heat summation.

N.B.: Experiments may be added to or omitted from the above list, if necessary.

Learning Outcomes: Upon completion of this course, the student will be able to

- determine the molecular mass by using a Victor Mayer's apparatus.
- calculate the equilibrium constant by titrimetric method.
- determine the rate of hydrolysis of an ester by titrimetric method.

- estimate the heat of solution from solubility measurement.
- find out the formula of a silverammine complex by titrimetric method.
- calculate the solubility product and investigate the effect of common ion.
- draw a phase diagram of phenol-water system and investigate the effect of added impurities.
- carry out steam distillation and verify the Hess's law by calorimetric method.

Books Recommended

1. Experimental Physical Chemistry, Daniel, Mathews and William (McGraw-Hill)
2. Experiments in Physical Chemistry, Bell and Newcombe.
3. Chemical Analysis, Laitonen
4. Vogel's quantitative Inorganic Analysis-Revised edition.

CH 321: CHEMISTRY OF NATURAL PRODUCTS

2 CREDITS

Learning Objectives: This course content will help the learners to

- acquaint the students with the fundamental ideas of natural products chemistry.
- understand extraction, isolation and structural elucidation of alkaloids, terpenoids, steroids and hormones, coloring materials and pheromones.
- explain the physical properties of alkaloids, terpenoids, steroids and hormones, coloring materials and pheromones.

Course Contents

1. **Introduction:** Definition, occurrence and importance of some natural products, primary and secondary metabolites.
2. **Alkaloids:** Occurrence, classification, extraction and purification of alkaloids, structural elucidation of morphine, ephedrine, adrenaline, nicotine, quinine and papaverine, Biosynthesis of alkaloids.
3. **Terpenoids:** Classification of terpenoids, isoprene rule, essential oils, isolation and purification of terpenoids, general methods of determining the structure of terpenoids, (i) acyclic monoterpenoids like myrcene, citral, (ii) monocyclic monoterpenoids like limonene, (iii) sesquiterpenoids like farnesol, biogenesis of terpenoids.
4. **Steroids and Hormones:** Introduction, nomenclature and functions, cholesterol and its effects in biological systems, steroid hormones, natural and synthetic hormones.
5. **Organic Coloring Materials:** A relationship between colour and constitution, anthocyanins, anthocyanidins, flavones, xanthenes and other materials, naturally occurring coloured

compounds, chlorophyll & hemoglobin.

6. Pheromones: Pheromones, their stereospecificity and actions in biological systems.

Learning Outcomes: Upon completion of this course, students will be able to

- describe the fundamentals of natural products chemistry.
- explain extraction, isolation, structural elucidation of alkaloids, terpenoids, steroids and hormones, coloring materials and pheromones.
- discuss the chemistry of some important natural products like alkaloids, terpenoids, steroids and hormones, coloring materials and pheromones.

Books Recommended

1. Chemistry of Organic Natural Products, Agarwal.
2. Organic Chemistry, Vol. 2, I. L. Finar, Longmans.
3. Natural Product Chemistry, K. B. G. Torsell.
4. Selected Organic Synthesis, I. Fleming.
5. An Introduction to the Alkaloids, G. A. Wawan,
6. Mono and Sesqui-terpenes, P. de Mayo.
7. Chemistry of the Alkaloids, S. W. Pelletier.
8. Natural Products Chemistry, P. S. Kalsi.

CH 322: ADVANCED STEREOCHEMISTRY**3 CREDITS**

Learning objectives: To provide the knowledge of

- isomers and concepts of configuration and conformation,
- assignment of (R) - and (S) - descriptions to stereogenic centers in chiral molecules
- provide in-depth knowledge on conformational analyses of fused and bridged ring compounds, proteins, nucleic acid and carbohydrates.

Course Contents

1. **Stereochemistry:** *Cis-trans* isomerism in C=C and C=N, cycloalkane; inter conversion of *cis-trans* isomers, physical properties: determination of configuration by chemical and physical methods; conformation of acyclic molecules: physical and spectral properties of diastereoisomers and conformers, conformation and reactivity, configuration: relative and absolute configuration, notation: R/S, D/L configuration determination; chemical interconversion, chemical correlation methods.
2. **Chiral and Prochiral Molecules:** Pro-R, Pro-S, homotopic and heterotopic ligands and faces. enantiotopic ligands (HCN addition) diastereotopic ligands and faces. Enzymatic oxidation-reduction, prostereoisomerism in biochemical reactions (citric acid cycle), stereochemistry of molecule synthetase reaction.
3. **Configuration and Conformation of Cyclic Compounds:** Three, four six-membered ring conformational analysis and di- and poly-substituted cyclohexanes, inositol, conformation and physical properties, reactivity in cyclohexane derivatives, Curtin-Hammet principle, cyclohexanones.
4. **Conformational Analysis of Biopolymers:** (i) Conformation of carbohydrates: anomeric effect, conformation of glycosides, starch, cellulose and effect of conformation on physical properties; (ii) Conformation of proteins, nucleic acids.
5. **Chirality in Molecules Devoid of Chiral Centres:** Atropisomerism, biphenyls, allenes, cyclic allenes, molecules with planar chirality, cyclophanes, annulenes; chromatographic resolution, kinetic resolution, enzymatic resolution.
6. **ORD and CD:** Optical rotatory dispersion (ORD), interpretation and application of ORD curve, circular dichroism (CD), application of CD, octant rule, α -haloketone rule.
7. **Fused Rings and Bridged Rings:** (i) Norbornanes-bridged rings (ii) strained carbocycles-Bredt's rule (iii) Fused rings: (a) Decalins (b) Hydrindanes (c) Steroid nucleus, bridged alkaloids.

Recommended Books

1. Stereochemistry of carbon compounds, E. I. Eliel, John Wiley and Sons.
2. Stereochemistry by Kagan, Edward Arnold,
3. Introduction to stereochemistry, Mislow, Benjamin.
4. Stereochemistry, conformation and Mechanism, P. S. Kalsi, Wiley Eastern Ltd.
5. Organic chemistry, Morrison and Boyd, Pearson.
6. Organic Chemistry, Vol. 2, I. L. Finar.

Learning Outcomes: After completing this course, students will acquire the knowledge of -

- i. advanced stereochemistry to analyze some selected organic molecules
- ii. the conformation of fused and bridged ring compounds.
- iii. distinguish the specific optical isomers of compounds devoid of chiral center

CH 323: ORGANIC REAGENTS AND SYNTHESES

2 CREDITS

Learning Objectives: Learning objectives of this course are to

- develop a knowledge base of synthetic organic reactions.
- provide in-depth understanding of structure reactivity principles in a variety of chemical structures.
- make the students capable of designing the strategies of complex molecular constructions.

Course Contents

1. **Oxidation Reaction:** Oxidation of hydrocarbon, alcohols. Allylic oxidation; Oxidation with peroxyacids, periodate, lead tetraacetate and SeO_2 .
2. **Reduction Reaction:** Catalytic hydrogenations, metal hydride reduction, reduction with dissolving metals.
3. **Synthesis Involving Interconversion and Protection of Functional Groups** (a) Interconversion of functional groups-transformation of alcohols, phenols, halogenocompounds, nitro compounds, acids and acid derivatives, (b) Protective groups: the strategy, protection of alcohols, diols, carboxylic acids, amino groups, carbonyl groups.
4. **Formation of Carbon-Carbon Bonds:** Preparation, structure, properties, reactions and applications of Grignard reagents, alkylated compounds of alkali groups (e.g., Li, Na), Organo-Copper compounds, Organozinc compounds, Organoaluminium compounds. Heck reaction, Suzuki reaction, Stille coupling, Sonogashira coupling, Hartwig reaction, Hypervalent iodines and their applications.
5. **Strategy in Synthesis:** Design of a synthesis, Initial consideration of the retrosynthetic approach, starting materials, yield and reaction; Synthesis of monofunctional and bifunctional

compounds: (a) One-group disconnection: disconnection of simple alcohols-compounds derived from alcohols, disconnection of simple olefins, ketones, (b) (i) Two group disconnections: 1,3-dioxygenated skeletons (ii) ‘Illogical’ two group disconnection - the 1,2-dioxygenation pattern; (c) Pericyclic reactions; (d) Heterocyclic compounds, strategy considering all possible disconnections.

- 6. Name Reactions:** Oppenheimer oxidation, Meerwein-Ponndorf-Varley reduction, Clemmensen reduction, Wolff-Kishner reduction, Wittig reaction, Baeyer-Villiger oxidation with mechanistic details.

Learning Outcomes: Upon completion of this course, students will be able to

- predict either the product or reactant from a given structure on the basis of the knowledge obtained from the study of the reactions covered e.g. C–C, C=C and C–X bond formations and eliminations, oxidations, reductions and protecting group transformations.
- design a retrosynthetic analysis using the disconnection approach.
- convert retrosynthetic analysis to a forward multistep synthesis.

Books Recommended

1. Some modern methods of Organic Synthesis (ISBN, Cambridge) by W. Carruther,
2. Organic Chemistry VOL. I (Longman group Ltd.) by I. L. Finar.
3. Modern Synthesis Reactions (W. A. Benjamin, New York) by H. O. House.
4. Organic Chemistry by Pine.
5. Organic synthesis: The disconnection approach (John Wiley & Sons) by Stuart Warren.
6. Synthesis and Chemistry of Agrochemicals by Don R. Baker, J. G. Fenyes and W. K. Moberg.
7. Organic Synthesis by Michael B. Smith.
8. Guidebook to Organic Synthesis by R. K. Mackie and D. M. Smith.

CHL 324: SELECTED TOPICS IN ORGANIC LABORATORY**2 CREDITS**

Learning Objectives: The course content will help the learners to

- expose *the* basic concepts and techniques related to estimation of functional groups.
- provide experimental knowledge on estimation of different functional groups.
- give idea about the purification of different types of organic compounds *using* different techniques.
- study the different effects of organic compounds.

Course Contents

1. **Estimation of Functional Groups:** (i) Estimation of carboxylic acid group present in an organic compound by iodometric titration. (ii) Estimation of hydroxyl and amino groups by acetylation. (iii) Estimation of carbonyl group by derivatization followed by gravimetric analysis. (iv) Estimation of aldehyde group by oxidation (Using Fehling/Benedict solution). (v) Estimation of adjacent hydroxyl groups by periodic oxidation.
2. **Purification of Organic Compounds:** Purification of organic compounds by recrystallization method, distillation and solvent extraction method.
3. **Studies of Some Organic Reactions:** a) Effect of solvents on S_N1 reactions. b) Effect of stereochemical aspects on esterification. c) Effect of structures with a common nucleophile leading towards nucleophilic additions. d) Cis-trans isomerism: conversion of maleic acid into fumaric acid and vice-versa.

N.B.: Experiments may be added to or omitted from the above list if necessary.

Learning Outcomes: Upon completion of this course, the student should be able to

- estimate the different types of functional groups.
- purify the organic compounds.
- realize the different effects on organic reactions.

Books Recommended

1. A text book Organic quantitative analysis, A. I. Vogel.
2. Chromatography: Published, IFS and ICAT.

CH 341: TRANSITION METALS AND COORDINATION CHEMISTRY**3 CREDITS**

Learning Objectives: The course content will help the learners to

- introduce the general characteristics of transition and inner transition metals and their comparison.
- demonstrate the rules and theories related to bonding, structure, stability, and magnetic properties of coordination compounds.
- convey knowledge on kinetics and reaction mechanism of coordination complexes.

Course Contents

- 1. Transition and Inner Transition Elements:** General characteristics of transition metals and inner transition metals, shapes of d and f orbitals, magnetism in transition metal chemistry, origin of paramagnetism and diamagnetism, magnetic susceptibility, Curie's law, techniques of magnetic measurements, Gouy balance, lanthanides and actinides: oxidation states, atomic and ionic radii of M^{3+} ions, magnetic properties of M^{3+} ions, lanthanide contraction, chemical reactivity of lanthanides, separation of lanthanide and actinide compounds, comparison between 3d and 4f block elements.
- 2. Bonding in Coordination Compounds:** Double salts and coordination compounds, coordination number, ligand types, Werner's coordination theory, limitations of Werner's postulate, Sidgwick's electronic concept, application of EAN rule, limitations of Sidgwick's concept, assumptions of valence bond theory (VBT), hybridization and geometry of complexes, inner orbital and outer orbital octahedral complexes, limitations of VBT, important features of crystal field theory (CFT), orbital splitting and electron spin, factors influencing the magnitude of $10dq$, spectrochemical series, crystal field stabilizing energies of d^n configuration ($n = 0$ to 10), magnetic moments, colour of transition metal complexes, distortion of octahedral complexes and Jahn-Teller theorem, limitations of CFT, ligand field theory (LFT), molecular orbital theory (MOT), MOT as applied to octahedral complexes, comparison of different theories.
- 3. Stability of Complex Compounds:** Stability, stepwise formation constants and overall formation constants, kinetic vs. thermodynamic stability, labile and inert octahedral complexes, factors affecting the stability of a complex, experimental determination of stability constant and composition of a complex.
- 4. Nomenclature and Isomers in Coordination Compounds:** Names of coordination compounds, use of abbreviated names, four and six coordination preferences, isomerism – structural and stereoisomerism in complex compounds, geometrical and optical isomerisms in 4- and 6- coordinate complexes, chirality.
- 5. Reactions and Mechanisms in Coordination Chemistry:** Substitution reactions in octahedral

complexes, types of substitution reactions, nucleophilic substitution reactions, association, dissociation and interchange mechanisms, factors affecting the rate of substitution reactions, acid and base hydrolysis reactions, the conjugate base mechanism, stereochemistry of octahedral substitution, substitution in square planar complexes, trans effect – theories of trans effect, uses of trans effect, substitution in tetrahedral complexes, fluxionality in coordination compounds.

Learning Outcomes: Upon completion of this course, the student should be able to

- explain the general properties of transition and inner transition elements
- illustrate the bonding, structure, stability and magnetism of coordination compounds.
- explain kinetics and mechanism of various types of reactions in coordination chemistry.

Books Recommended:

1. Advanced Inorganic Chemistry, F. A. cotton G. Wilkinson, C. A. Murillo and M. Bochman.
2. Inorganic Chemistry, James E. Huheey, 4th ed., Haper Collins.
3. Inorganic Chemistry, G. L. Miessler and D. A. Tarr.
4. An Introduction to Inorganic Chemistry, K. F. Purcell and J. C. Kotz, Saunders Golden.
5. Inorganic Chemistry, D. F. Shriver, P. W. Atkins and C. H. Langford.
6. Chemical Applications of Group Theory, F. A. Cotton.
7. Infrared and Raman Spectra of Inorganic and Coordination Compounds, K. Nakamoto.
8. Mechanisms of Inorganic reactions by F. Basolo and R. G. Pearson.
9. Inorganic Reaction Mechanisms, M. L. Tobe, Nelson.

CH 342: INORGANIC PROCESS INDUSTRIES

2 CREDITS

Learning Objectives: The course content will help the learners to

- give a general understanding of classification, properties, uses and industrial manufacturing process of few important materials in Bangladesh.
- gain knowledge on analysis and quality control of various industrial products.

Course Contents

1. **Fundamentals in the Development of Chemical Industries:** General ideas about unit processes and unit operations, raw materials, process design, commercial energy sources, skilled manpower, catalysts, water as the basic process fluid, heat transfer, mass transfer, separation processes, concepts of consumption, production, and market evaluation, the balance of supply and demand, safety, environmental considerations, site and technology selection criteria, cost-benefit analysis.

2. **Chlor-alkali Industries:** Raw materials, manufacture of caustic soda, soda ash, sodium bicarbonate, chlorine, bleaching powder, sodium chlorite, environmental hazards of these chemicals.
3. **Fertilizer Industries:** Plant nutrients, classification of fertilizers, natural inorganic fertilizers, nitrogen fixation, artificial fertilizers, manufacture of ammonia, urea, ammonium sulfate, ammonium nitrate, action of urea as fertilizer, potassium fertilizer, calcium phosphate and other phosphatic fertilizers, potassium fertilizer, NPK fertilizer.
4. **Cement Industries:** Portland cement, raw materials, important process parameters for manufacturing a good cement clinker, methods of manufacturing Portland cement, sequence of operations, additives for cement, properties of cement, testing of cement, setting of cement, other types of cement, manufacture of gypsum, Plaster of Paris.
5. **Glass and Ceramic Industries:** Properties of glass, raw materials and fundamentals of glass industries, methods of manufacture, special glasses, ceramics, properties of ceramics, basic raw materials, manufactures of ceramics.
6. **Iron and Steel Industry:** Fundamentals of metallurgy, ores of iron, three commercial forms of iron, construction and operation of blast furnace, reactions in blast furnace, by product in blast furnace, classification of steel, steel manufacturing processes, effects of impurities on steel, phases in Fe-C system.

Learning Outcomes: Upon completion of this course, the student should be able to

- *Describe the properties, classification, uses and the industrial manufacturing methods of fertilizers, cement, glass and ceramic; and caustic chlorine products.*
- *Discuss the ores processing of iron and steel.*

Books Recommended

1. Chemical Process Industries, R. N. Shreve and J. A. Brink, Jr., McGraw-Hill Inc.
2. Industrial Chemistry, B. K. Sharma.
3. Reagel's Hand Book of Industrial Chemistry, J. A. Kent edited, Van Nostrand.
4. Chemical Process Industries, G. T. Austin edited, McGraw-Hill.
5. Inorganic Medicinal and Pharmaceutical Chemistry, J. H. Block and E. B. Roche.
6. Environmental Chemistry Vol. I-III, H. J. M. Bowen.

CHL 343: INORGANIC SYNTHESIS AND CHARACTERISATION**2 CREDITS**

Learning Objectives: The course content will help the learners to

- impart knowledge on preparation and characterization of some inorganic compound.
- convey knowledge on characterization by chemical analysis, infrared spectroscopy and magnetic measurement.

Course Contents

1. Recrystallization of NaCl crystals from crude NaCl and its characterization.
2. Preparation of FeSO₄.7H₂O and its characterization including estimation of water of crystallization and determination of Fe³⁺ as impurity, if any.
3. Preparation of CuSO₄.5H₂O from metallic copper and its characterization by elemental analysis, IR and UV-visible spectra, and thermal analysis.
4. Synthesis of [Cu(NH₃)₄]SO₄.H₂O from CuSO₄.5H₂O and its investigation by infrared spectrometer.
5. Preparation of [Co(NH₃)₆]Cl₃ and its characterization by chemical analysis, infrared spectroscopy and magnetic measurement.
6. Preparation and characterization of tris(thiourea)copper(I) chloride, [Cu(NH₂CSNH₂)₃]Cl.
7. Synthesis of an ethylenediamine complex of cobalt and its characterization by infrared and ¹H NMR spectroscopy.
8. Preparation and investigation of potassium tris(oxalato)ferrate(III), K₃[Fe(C₂O₄)₃].
9. Preparation and characterization of the optical isomers of tris(ethylenediamine)cobalt(III) iodide, [Co(en)₃]I₃.
10. Synthesis and characterization of a saccharin complex.
11. Spectrophotometric determination of Cr₂O₇²⁻ and MnO₄⁻ concentration from their solution.
12. Preparation of anhydrous AlCl₃ and anhydrous FeCl₃.

Learning Outcomes: Upon completion of this course, the student should be able to

- understand the characterization by chemical analysis, infrared spectroscopy and magnetic measurement.
- explain synthesis and characterization of a complex.

Books Recommended

1. A Text Book of Quantitative Inorganic Analysis, A. I. Vogel.
2. Microscale Inorganic Chemistry, Z. Szafran, R. M. Pike, and M. M. Singh,
3. Inorganic Experiments, J. D. Woollins edited, VCH.

CH 361: CHEMICAL SPECTROSCOPY**3 CREDITS**

Learning Objectives: This course content will help the learners to

- realize the interaction between electromagnetic radiation and matter.
- achieve knowledge on the fundamental principles of spectroscopic techniques.
- attain the concepts of absorption, emission and chemical shift.
- understand the basics of vibrational, rotational and other types of transitions.
- study the fates of photoexcited species.

Course Contents

- 1. Electromagnetic Radiation:** The nature of electromagnetic radiation, emission and absorption spectra; spectrometers; basic components of dispersive spectrometers; modulation technique: transmittance and absorbance, Beer-Lambert law: molar absorption cross section, Representation of spectra; spectral peaks; intensities, width and resolution; signal to noise ratio and signal averaging, Fourier transform technique and its advantages.
- 2. Rotational Spectroscopy:** Rotation of molecules and their classification. Interaction of rotating molecules with radiation. Microwave spectrometer. Rotational energies of linear rotors. Distribution of molecules and rotational spectra. Centrifugal distortion. Effect of isotopic substitution. Stark effect and its use in microwave spectrometers. Determination of molecular geometry from microwave spectra.
- 3. Infrared Spectroscopy:** Vibration in molecules; normal modes, harmonic and anharmonic. Potential-energy diagrams. Morse equation, vibrational energy, dissociation energy of diatomic molecules, population of vibrational levels. Transition probabilities. Fundamental, overtone and hot band transitions. Combination and difference bands, Fermi resonance. Vibration-rotation spectra of gaseous molecules. P, Q, and R branches, infrared spectra of polyatomic molecules. Characteristic group vibrations and skeletal vibrations, shifts in group frequencies, Techniques: radiation sources, optics, monochromators, sample holders, detectors for infrared spectrometers. Handling of samples: gaseous, liquid and solid samples. Principle of FTIR spectrometer and its advantages.
- 4. Raman Spectroscopy:** Raman effect, classical theory of Raman scattering, criterion of Raman activity, Raman spectrometers; use of laser in Raman spectroscopy, vibrational and rotational Raman spectra, use of polarized light, applications of Raman spectroscopy.
- 5. Ultraviolet-visible Spectroscopy:** Electronic states of molecules. Spectra of simple gaseous diatomic species and their vibrational coarse structure. Franck-Condon principle and intensities of spectral lines. Dissociation energy; pre-dissociation spectra of species in condensed phase.

Various electronic transitions in organic and inorganic species. Width of electronic bands, effect of solvent on band width and band position. Chromophores, bathochromic and hypsochromic shifts. Auxochromes.

6. **NMR Spectroscopy:** Nuclear spin resonance, Larmor/precessional frequency, Effect of magnetic field on the energies of spinning nuclei, Electron density at the nucleus; the chemical shift; δ and τ -scale for chemical shift; Factors affecting the chemical shift, the coupling of nuclear spins, the coupling constant; exchange phenomenon; NMR spectrum of simple compounds. The NMR spectrometer.
7. **ESR Spectroscopy:** Effect of magnetic field on the energies of spinning electrons, Larmor/precessional, g-factor, hyperfine splitting, determination of electron density from ESR spectroscopic studies. The ESR spectrometer.

Books Recommended

1. Fundamentals of Molecular Spectroscopy, C. N. Banwell & E. M. McCash. McGraw Hill, N.Y.
2. Introduction to Spectroscopy, Donald L. Pavia, Gary M. Lampman, George S. Kriz.
3. Introduction to Molecular Spectroscopy, G. Barrow.
4. Molecular Structure and Spectroscopy, G. Aruldas, Prentice-Hall of India.
5. The Infrared Spectra of Complex Molecules, Bellamy, Chapman and Hall.
6. Ultraviolet and Visible Spectroscopy, Rao.
7. Molecular Spectroscopy, Raymond Chang.

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

- i. know the absorption and emission of radiation, region of spectrum and quantization of energy
- ii. determine the bond length of diatomic molecule, rotational constant (b), ratio of population in different energy states and resonance frequency.
- iii. distinguish between the nuclear spin and electron spin resonance.
- iv. understand the principles of microwave, IR, NMR, ESR spectroscopy and explain the spectrum.
- v. explain the allowed transition between vibrational, rotational, electronic energy levels for atom/molecules.
- vi. apply microwave, IR, Raman, UV-Visible, NMR and ESR spectroscopy for chemical analysis.

CH 362: CHROMATOGRAPHIC METHODS**2 CREDITS**

Learning objectives: To provide theoretical knowledge

- (i) In the field of chromatography, as one of the most modern analytical and separation techniques.

Course Contents

1. Chromatography: Overview, retention behavior, efficiency, selectivity, resolution, chromatographic theory, measured chromatographic parameters, evaluation methods, and classification of chromatography.

2. Liquid Chromatography: Types of liquid chromatography.

2.1 Column Chromatography: Column selectivity, efficiency, capacity factor, etc.

2.2 Ion-Exchange Chromatography: Ion-exchange resin, types of resins and their structure and properties, factors affecting the ion-exchange-equilibria, eluting solvents, effect of pH, effect of complexing agents, and application of ion-exchange chromatography.

2.3 High-Performance Liquid Chromatography: The HPLC system, particle size and support material, filtration and degassing, HPLC columns, solvent requirements, solvent pumping systems, injection systems, HPLC detectors, applications.

3. Planar Chromatography: Theories and mechanism of PC and TLC, nature of stationary phases, general properties required of a mobile phase, development of the chromatograms, location of spots, superiority of TLC, analytical applications.

4. Gel Chromatography: Mechanism of gel chromatography, advantages of gel chromatography, technique of gel chromatography, applications of gel chromatography.

5. Gas Chromatography: Principles, GC columns, selection of materials and column design, stationary phases, carrier gas, sample injection system, general properties of detectors, detector types, scope of gas chromatography.

6. GC-MS: Combined technique for chemical analysis.

Learning Outcomes: Upon successful completion of this course, students will be able to

- understand the importance of chromatographic separation.
- apply the chromatographic techniques for qualitative and quantitative analysis in various fields of chemical industry, pharmaceutical industry, the environment and other analytics.
- demonstrate the independence of the appropriate optimization of chromatographic methods.

Books Recommended

1. Chromatographic Method, Braithwaite and Smith.
2. Gas and liquid Chromatography in Analytical Chemistry, Roger. M. Smith.
3. Introduction to Chemical Analysis, R. D. Braun.
4. Instrumental Methods of Chemical Analysis, Ewing.

CHL 363: INDUSTRIAL CHEMISTRY LABORATORY**2 CREDITS**

Learning Objectives: This course content will help the learners to

- give a general understanding of classification, properties, uses and industrial manufacturing process of few important materials.
- gain knowledge on analysis and quality control of various industrial products.

Course Contents

1. **Water Analysis:** Analysis of water for temporary and permanent hardness, total suspended solids, chloride content, dissolve oxygen, arsenic and lead.
2. **Industrial Materials:** Analysis of an iron and a calcium compound, analysis of coal for sulfur and quality specifications in terms of carbon content and inorganic residues.
3. **Environmental samples:** Air particulate matters for total suspended solids, analysis of lead, calcium, copper and sulfur, air pollutants: SO_x and NO_x levels in air.
4. **Metals and Alloys:** Analysis of steel for manganese and sulfur.
5. **Analysis of Fats and Oils:** Fats and oil analysis for acid value, iodine value and saponification value.
6. **Analysis of Carbohydrates:** Analysis of cane sugar for glucose by Fehling's solution and Benedict solution methods, analysis of molasses for glucose content.
7. **Soaps and Detergents:** Analysis of soap for total acid and alkali, and free acid or free alkali values for quality control.
8. **Food and Drinks:** Analysis of milk for sugar and protein.
9. **Analysis of Pharmaceutical Products:** Assay of L-ascorbic acid, vitamin C-tablets, aspirin and aspirin tablets.

Learning Outcomes: Upon completion of this course, the student will be able to

- Analyze the water samples, air samples, carbohydrates, soap and detergents.
- Determine the acid value, iodine value and saponification value of oils and fats.

- Analyze various industrial products.

Books Recommended

1. A Text Book of Quantitative Inorganic Analysis, A. I. Vogel.
2. Comprehensive Practical Organic Chemistry, V. K. Ahluwalia and R. Aggarwal.
3. Preparative Methods of Polymer Chemistry, W. R. Sorenson and T. W. Campbell.
4. Standard Methods for the Examination of Water and Wastewater, APHA-AWWA-WPCF, Washington.

CHL 364: BASIC COMPUTERS AND COMPUTATIONAL CHEMISTRY LABORATORY 2 CREDITS

Learning Objectives: This course content will help the learners to

- impart skill on writing chemistry texts involving chemical formulae and draw structures of chemical compounds.
- analyze experimental data.
- study *the properties of molecules* by computer simulation.

Course Contents

Part A

1. Introduction to Windows and MS-DOS.
2. Introduction to Microsoft Word. Writing chemistry texts involving chemical formulae, superscripts, subscripts, symbols.

Part B

1. Advanced word processing-Tabs, tables, use of the equation editor in chemistry.
2. Two-dimensional chemical structure drawing using Chem-Window.
3. Microsoft Excel/Origin-Chemical spreadsheets (use of the function wizard, formulae) and graphs in chemistry (line graphs and scatter plots).

Part C

1. Databases using Access.
2. Use of Power Point.
3. Molecular Structure Drawing using Chemdraw 2D and 3D.
4. Use of Internet. During the progress of the course, use of new software will be encouraged depending on availability.

Part D

1. Molecular structure drawing using Chemdraw, Chemsketch and Chemwindow.
2. Data analysis using Microsoft Excel, Origin, Igor and Sigma plot. .
3. Computer Aided Molecular Design: Protein Structure Basics (Amino Acids, Peptide Formation, Dihedral Angles, Hierarchy, Secondary and Tertiary Structures); Determination of Three-Dimensional Protein Structure; Visualization, Comparison, and Classification; RNA Structures (Types, Structure Prediction).
4. Visualization softwares: GaussView, Molekel, etc.

N.B.: Experiments may be added to or omitted from the above list if necessary.

Learning Outcomes:

Upon completion of this course, the student will be able to

- *Organize and interpret collected experimental data.*
- *Draw chemical structures*
- *Compare and explain the properties of a molecule determined both by experimentally and by computer simulation.*

Recommended Books

1. Microsoft Office, 97/2000, Mahbubur Rahman, Cistech publications, 38/3 Bangla Bazar, Dhaka.
2. SAMS Teach Yourself Microsoft Office 2000 in 21 days, Laurie Ulrich, Techmedia, New Delhi-2.
3. Bruce A. Hallberg and Joe Casad, Windows 98, Techmedia, 20 Ansari Road, New Delhi-2.

CH 371: QUANTUM CHEMISTRY AND STATISTICAL MECHANICS**3 CREDITS**

Learning Objectives: This course content will help the learners to

- illustrate the failures of classical mechanics.
- acquire knowledge in development of quantum mechanics.
- get idea about some principles and postulates of quantum mechanics.
- study the applications of quantum mechanics.
- learn probability distribution of particles, partition function and quantum statistics.

Course Contents

1. **Classical Mechanics:** Failures of classical mechanics. Black-body radiation, heat capacities of solids, photoelectric effect, the Compton effect, atomic spectra, Planck's quantum theory, Einstein's explanation of photoelectric effect, de Broglie's postulate, Heisenberg's uncertainty principle, wave equation.
2. **Time Independent Schrodinger Equation and Stationary State:** Interpretation of the wave function: normalization of the wave functions. Orthogonality and completeness of the wave function. Significance of wave functions.
3. **Operators and Observables:** Constitution of quantum mechanical operator, some important operators: Hamiltonian operator, Laplacian operator, operator algebra, eigen functions, eigen values, eigen value equation, expectation values.
4. **Application of Quantum Mechanics:** Translational motion, particle in a box, properties of solutions and the consequences, vibrational motion, one-dimensional harmonic oscillator: the formal solution, the energy levels, the wave functions, properties of the solutions, rotational motion: rotation in two dimensions, the formal solution, significance and application.
5. **Structure of Hydrogen and Hydrogen-Like Atom:** The formal solution of the Schrodinger equation; the separation of the R, Θ and Φ equations, total wave functions of the hydrogen and hydrogen-like atoms, probability density and radial distribution function, atomic orbitals and their shapes, orthonormality of atomic orbitals, approximation methods, variation principle, perturbation theory.
6. **Statistical Mechanics:** Basic concepts, macroscopic system, distribution of molecules, configuration, population, weight, most probable configurations, Boltzmann distribution, molecular partition function; internal energy of a system; the canonical ensemble; Fermi-Dirac

and Bose-Einstein statistics, evaluation of partition functions, calculation of thermodynamic functions, applications of statistical mechanics, mean energies and the equipartition principle, heat capacities of solids, Einstein and Debye equations, chemical equilibrium: statistical treatment, evaluation of equilibrium constants, Stirling's approximation.

Learning Outcomes: Upon completion of this course, the student should be able to

- understand the failure of classical mechanics, black body radiation, photoelectric and Compton effects, Heisenberg's uncertainty principle, Schrodinger wave equations, eigen values and eigen functions, and postulates of quantum mechanics.
- realize probability distribution of particles in various energy states, most probable distribution, relation between probability and thermodynamics, Maxwell-Boltzmann distribution law.
- understand partition functions and its physical significances, relation between partition functions and thermodynamic functions, statistical expression for equilibrium constant.
- compare and contrast Maxwell-Boltzmann statistics, Bose-Einstein statistics and Fermi-Dirac statistics.
- differentiate between Einstein and Debye theories of specific heat.
- analyze the values of partition function, equilibrium constant, specific heat of solids etc.

Books Recommended

1. Quantum Mechanics in Chemistry by M.W. Hanna.
2. Quantum Chemistry by McCurry.
3. Quantum Chemistry by P. W. Atkins, Oxford University Press.
4. Introduction to quantum mechanics by A. K. Chanda.
5. Physical Chemistry by P.W. Atkins (Oxford).
6. Molecular quantum mechanics by P.W. Atkins, Oxford University Press.
7. Quantum chemistry, (2nd. ed.) by I.N. Levine, Allyn and Bacon, Boston.

CH 390: VIVA VOCE

2 CREDITS