



# Curriculum

for  
Bachelor of Studies  
in  
Chemistry

Effective from 01-01-2007

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## INTRODUCTION

Chemistry is a central science which helps to understand the origin of life and suggest ways to use non-living things for giving comfort to life. To train the young generation and to direct their approach so that they accomplish this task easily, it is necessary to make the students understand the principles underlying the composition, structure and properties of substances alongwith the transformation that they undergo. It is therefore obvious that chemical orientation cannot be imparted in isolation and has to be developed through a cocktail of physics and biology on one hand and engineering and applied sciences on the other. The Department of Chemistry, University of Karachi is well equipped for pursuing this goal having skilled and proficient faculty, well equipped laboratories and other infrastructure.

The Bachelor of Studies (BS) in Chemistry is planned to prepare the students to face the challenges of 21<sup>st</sup> century. This syllabus encompasses the growing needs of the young and competent scholars, to equip them with necessary techniques and knowledge so that they may achieve their true vocation in life. Department of Chemistry imparts professional and academic excellence to young people, which trains them to adapt and innovate to ensure their success in various fields of life in the world of tomorrow. Unlike other similar institutions of Karachi whose degrees are only Organic Chemistry specific, it caters for all the disciplines of Chemistry i.e. Inorganic, Organic, Physical and Analytical Chemistry, while in each of these disciplines additional specializations like Pharmaceutical chemistry, Polymer chemistry and many others are offered.

### **Background**

The University of Karachi was established in 1951 under a charter of the central government. Till 1959 it was housed in rented buildings situated in a congested area at Princesses Street. In 1960 it moved to the present campus sprawling over an area of nearly two square miles. The campus has since been growing steadily. The Department of Chemistry is one of the oldest departments of University of Karachi. When the university was shifted to its present location, the department occupied one of the few newly constructed buildings and is still housed there for the last 47 years.

Over 50 years the department has awarded more than 7000 B.Sc (Hons) and M.Sc degrees. Besides, above 100 research scholars have completed their M.Phil and Ph.D degrees. There are approximately 35 colleges imparting education in Chemistry at undergraduate level whose syllabi and examinations are supervised by this department.

The Department of Chemistry is a dynamic, innovative and self-motivated institution dedicated to the high quality, effective training and maintaining its degree in confirmatory with the international accepted standards. Through its 40 qualified academic faculty, it provides excellent environment for graduate and post graduate education in all the disciplines. The department was launched through Professor Dr. Sadik Antonof, the founder head of the department. Professor Dr. Muhammad Saeed Arayne is the present Chairman of the department. In the presence of very modest facilities the department has accomplished respectable goals. The research activities of the department have been commendable in comparison to other universities of the country. The department has organized and hosted National and International Chemistry Conferences

In recent years many candidates of this department have completed M.Phil and Ph.D and most of them are now working in renowned and esteemed institutions and industries. Every year the researchers of the department publish more than 50 research papers and books. Currently there are over forty teachers in the faculty, twenty four of them holding PhD degrees. Many of our teachers and students have presented their research in international conferences/seminars and most of them are pursuing vigorous research programs within the limited resources.

## Comparison of B.Sc. (Hons) & M.Sc Courses with BS Courses

Old Course No	New Course No	Course title
<b>BS Chemistry First Year</b>		
<b>Semester I</b>		
CHM-305	CHM-311	Inorganic Chemistry
CHM-300	CHM-301	General Chemistry
CHM-302	CHM-302	Organic Chemistry
—	IS-300.1	Islamic Studies (Compulsory)
—	E-300.1	English (Compulsory)
<b>Semester II</b>		
CHM-304	CHM-312	Organic Chemistry
CHM-300	CHM-301	General Chemistry
CHM-302	CHM-302	Organic Chemistry (s)
—	PS-300.2	Pakistan Studies (Compulsory)
—	U-300.2	Urdu/Sindhi/Natural Science (Compulsory)
<b>BS Chemistry Second Year</b>		
<b>Semester III</b>		
CHM-401	CHM-411	Physical Chemistry
CHM-402	CHM-412	Organic Chemistry
CHM-405	CHM-401s	Physical Chemistry
CHM-406	CHM-402s	Inorganic Chemistry
—	F.M-400.1	Functional Maths (Compulsory) (for the students of Biological Sciences)
—	Bio-400.1	Biology (Compulsory) (for the students of Physical Sciences)
—	E-400.1	English-II (Compulsory)
<b>Semester IV</b>		
CHM-403	CHM-421	Physical Chemistry
CHM-404	CHM-422	Inorganic Chemistry
CHM-405	CHM-401s	Physical Chemistry
CHM-406	CHM-402s	Inorganic Chemistry
—	F.M-402.1	Functional Maths (Compulsory) (for the students of Biological Sciences)
—	Bio-402.1	Biology (Compulsory) (for the students of Physical Sciences)
—	C-400.1	Computer Applications (Compulsory)

Old Course No	New Course No	Course title
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### BS Chemistry Third Year

#### Semester V

—	ISS-501	Introduction of Social Sciences
CHM-501	CHM-511	Analytical Chemistry
CHM-502	CHM-521	Industrial Chemistry
CHM-503	CHM-531	Inorganic Chemistry
CHM-504	CHM-541	Organic Chemistry
CHM-505	CHM-551	Physical Chemistry

#### Semester VI

—	CS-502	Communication Skills
CHM-506	CHM-512	Analytical Chemistry
CHM-507	CHM-522	Industrial Chemistry
CHM-508	CHM-532	Inorganic Chemistry
CHM-509	CHM-542	Organic Chemistry
CHM-510	CHM-552	Physical Chemistry

### BS Fourth Year

#### Analytical Chemistry

#### Semester VII

—	CD-601	Community Development (Compl.)
CHM-642	CHM-611	Statistics for Chemists and Introduction to Environmental Analytical Chemistry
CHM-641	CHM-621	Thermodynamics & Solution Chemistry
CHM-646	CHM-631	Spectroscopy-I
CHM-649	CHM-641	Instrumental Methods of Chemical Analysis (Lab Course)
CHM-644	CHM-651	Potentiometry and Amperometry (Lab Course)

Old Course No	New Course No	Course title
<b>Semester VIII</b>		
—	ECO-602	Economics (Compl.)
CHM-640	CHM-612	Electronics & Mass Spectrometry
CHM-645	CHM-622	Electroanalytical Chemistry and Introduction to Analytical Separation
CHM-647	CHM-632	Spectroscopy-II
CHM-648	CHM-642	Classical Methods of Chemical Analysis (Lab Course)
CHM-643	CHM-652	Clinical Methods of Analysis and Environmental Analytical Chemistry (Lab Course)
—	CHM-622.1	Pharmaceutical Chemistry (Optional, in lieu of 622)

### Organic Chemistry

<b>Semester VII</b>		
—	CD-601	Community Development (Compl.)
CHM-610	CHM-613	Spectroscopic Studies of Organic Molecules
CHM-611	CHM-623	Advanced Organic Reaction Mechanisms-I
CHM-612	CHM-633	Pharmaceutical Chemistry
CHM-613	CHM-643	Quantitative Organic Analysis (Lab course)
CHM-614	CHM-653	Natural Products Lab
CHM-633	CHM-633.1	Advanced Chemistry of Alkaloids
CHM-631	CHM-633.2	Chemistry of organic Nitrogen Compounds Excluding alkaloids
<b>Semester VIII</b>		
—	ECO-602	Economics (Compl.)
CHM-615	CHM-614	Advanced Organic Reactions
CHM-616	CHM-624	Advanced Organic Reaction Mechanisms-II
CHM-617	CHM-634	Stereochemistry
CHM-618	CHM-644	Organic lab. preparations
CHM-619	CHM-654	Qualitative Organic Analysis
CHM-634	CHM-634.1	Modern Trends in Organic Synthesis
CHM-630	CHM-634.2	Organic Reactions and Molecular Orbital Symmetry

—	CHM-634.3	Polymers, Food and cosmetic Chemistry
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### Physical Chemistry

#### Semester VII

—	CD-601	Community Development (Compl.)
CHM-620	CHM-615	Thermodynamics & Electrochemistry
CHM-621	CHM-625	Polymer Chemistry
CHM-622	CHM-635	Quantum Mechanics and spectroscopy
CHM-623	CHM-645	pH-metry and Potentiometry LABS
CHM-624	CHM-655	Spectroscopy labs.

#### Semester VIII

—	ECO-602	Economics (Compl.)
CHM-625	CHM-616	Radiation Chemistry and Photochemistry
CHM-626	CHM-626	Chemical Kinetics
CHM-627	CHM-636	Radiochemistry
CHM-628	CHM-646	Chemical Kinetics (Practicals)
CHM-629	CHM-656	Conductometry (Labs)

### Inorganic Chemistry

#### Semester VII

—	CD-601	Community Development (Compl.)
CHM-600	CHM-617	Kinetics & Mechanism of Inorganic Reactions
CHM-601	CHM-627	Characteristics of metal complexes
CHM-602	CHM-637	i) Material Science and Marine Chemistry
CHM-603	CHM-647	Inorganic Synthesis and Characterization Using Statistical Methods (Lab course)
CHM-604	CHM-657	Classical Methods of Analysis (Lab course)

**Semester VIII**

—	ECO-602	Economics (Compl.)
CHM-605	CHM-618	Applications of Instrumental Techniques
CHM-606	CHM-628	i) Organometallic Complexes and Inorganic Industrial Chemistry
CHM-607	CHM-638	Bio-inorganic Chemistry
CHM-608	CHM-648	Synthesis, Analysis & Characterization of Transition Metal Complexes (Lab course)
CHM-609	CHM-658	Instrumental Methods of Analysis (Lab course)
CHM-657	CHM-638.1	Industrial Environmental Chemistry

**BS CHEMISTRY FIRST YEAR  
SEMESTER-I**

**CHM-311 INORGANIC CHEMISTRY**

Credit Hours: (2+1)

**ATOMIC STRUCTURE**

Development of theories for atomic structure, discovery of fundamental subatomic particles. Bohr's model for Hydrogen, Line spectrum. Introduction to quantum mechanics, wave Mechanics, Quantum numbers and their significance.

**PERIODIC TABLE**

Electronic configuration and periodic table, periodicity, group trends in atomic and ionic radii. Trends in ionization energies, electro negativity, ionization potential, electron affinity, oxidation potentials, electrode potential. magnetic properties, Para and diamagnetisms.

**CHEMICAL BONDING IN s AND p BLOCK ELEMENTS**

Effective atomic number and shielding constant, types of chemical bonds. Ionic bond, covalent bond. The concept of hybridization and its applications. Theories of chemical bonding. Valence Bond theory and Molecular Orbital theory. Lattice energy and Born Haber cycle of Ionic compounds, related numericals.

**CHEMICAL REACTIONS IN AQUEOUS SOLUTION**

Acid base reactions, strong weak acids and bases, Net Ionic equations for acid base interactions. Precipitation reactions,  $K_{sp}$  values. Redox reactions, balancing redox equations.

**HALOGENS**

General properties of their reactions, Oxyacids, and their properties Interhalogen Compounds.

**ZERO GROUP**

General Properties of Zero group elements, Preparation properties of helium compounds of xenon.

## **ENVIRONMENTAL CHEMISTRY**

Composition of the atmosphere. Chemical reactions taking place in the atmosphere. Industrial and domestic effluents and their treatments. Solid waste disposal technologies. Ozone in the upper atmosphere, depletion of the ozone layer. Pollution and types of pollutants (solids, liquids and gases), determination of pollutants. Sulfur compounds and acid rain, carbon monoxide, nitrogen oxides and photochemical smog. Water vapors, carbon dioxide, and climate.

## **METALLURGY**

Principles of metallurgical operations. Metallurgy of iron and Steel, Purification of metals

## **PRACTICALS**

### **QUALITATIVE ANALYSIS**

Acid radicals, group tests, preliminary tests, Confirmatory tests. Basic radicals, group separation, radical analysis. Confirmative tests.

## **BOOKS RECOMMENDED**

1. Whitten KW, Davis RE, Peck LM and Stanley G "General Chemistry" 7<sup>th</sup> Ed (2004) Thomas Learning.
2. Ralph PH and Harwood WS "General Chemistry: Principles and Modern Applications" 8<sup>th</sup> Ed (2002) Prentice Hall
3. Whitten KW, Davis RE, Peck LM and Stanley G "General Chemistry with Qualitative Analysis" 6<sup>th</sup> Ed (2002) Thomas Learning.
4. Manahan SE "Environmental Chemistry" 6<sup>th</sup> Ed (1994) Lewis Publisher.
5. Dara SS "Environmental Chemistry and Pollution Control" 1<sup>st</sup> Ed (1993) S. Chand & Co. Ltd. Delhi
6. Chang R "Chemistry" 7<sup>th</sup> Ed (2002) McGraw Hill, Higher education Commission
7. Atkins PW and Shriver DF "Inorganic Chemistry" 3<sup>rd</sup> Ed (1999) W.H. Freeman & Co
8. Vogel AI and Svehla G "*Vogel's Qualitative Inorganic Analysis*" 7<sup>th</sup> Ed (1997) Prentice Hall

## SEMESTER-I/II

### CHM-301(Minor) GENERAL CHEMISTRY

*Credit Hours: (3+0)*

#### **ATOMIC STRUCTURE**

Discovery of fundamental subatomic particles. Bohr's Hydrogen atom, Line spectrum and related problems. Introduction to quantum and Wave Mechanics, Quantum Numbers and related problems.

#### **PERIODIC TABLE**

Electron Configuration and Periodic Table, Periodicity, Group trends in atomic and ionic radii. Group trend in ionization energies, Electronegativity, Ionization Potential, Electron affinity, Oxidation potential, Electrode Potential, Magnetic Properties, Diamagnetism and Paramagnetism.

#### **CHEMICAL BONDING IN s AND p BLOCK ELEMENTS**

Different types of Chemical Bonds. Ionic bond, covalent bond. Hybridization and its Application. Theories of Chemical bonding, Valence Bond theory and Molecular Orbital Theory. Lattice energy and Born Haber Cycle of ionic Compounds.

#### **HALOGENS AND ZERO GROUP ELEMENTS**

General Properties of Halogens. Halides and their reactions. Interhalogen Compounds. General Properties of Zero group elements. Special Properties of Helium Compounds of xenon, their preparations and structure

#### **ENVIRONMENTAL CHEMISTRY**

Composition of the atmosphere. Chemical reactions taking place in the atmosphere. Industrial and domestic effluents and their treatments. Solid waste disposal technologies.

#### **PROPERTIES OF MATTER (GASES, LIQUIDS, AND SOLIDS)**

**Gases:** Vander Waal's modification of general gas equation, critical point and liquefaction of gases, the law of corresponding states. Kinetic energy and temperature. The law of equipartition of energy, Mean free path, collision number and collision diameter. Dipole dipole interactions. Induction effect and hydrogen bonding.

**Liquids:** Physical properties of liquids, surface tension, viscosity, refractive index. Phase changes, heating curves, Critical temperature, vapor pressure, boiling point, and volatility.

**Solids:** The symmetry of crystals. Symmetry, classification of crystals and unit cells. Arrangement of unit cells. Bonding in solids (covalent network solids, ionic solids, and metallic solids)

### **PROPERTIES OF SOLUTIONS**

Solution process: Energy changes and solution formation, concentration units, Raoult's law of ideal solution. Colligative properties and its application (elevation of boiling point, depression of freezing point, lowering of vapor pressure, osmosis, osmotic pressure), Ideal and non ideal solutions, binary mixtures.

### **BASIC CONCEPTS OF ORGANIC CHEMISTRY**

Bonding in organic compounds. Relation of structure with physical properties. Reactivity of organic compounds. Oxidation states of carbon. Structure and stability of reactive intermediates (carbocation, carbanion, free radical and carbene). Electrophiles & Nucleophiles. The arrow notation in reaction mechanism. Types of reactions; Substitution, Elimination, addition. Factors effecting reactions (reaction mechanism), electronic effects (Resonance & Mesomeric effects), steric effects, Solvent effects, Structural effects.

### **ACID BASE CONCEPT OF ORGANIC CHEMISTRY**

Theories of acids and bases. Lowery & Bronsted and Lewis theory of acids and bases & dissociation constant. Structure of carboxyl, phenol and their ions. Salt formation. Factors effecting strength of acids; electronic effects, steric effects, solvent effects, substituent effect. Basic compounds; aliphatic amines, aromatic amines, heterocyclic nitrogenous compounds. Factors effecting strength of bases; electronic effects, steric effects. effects of hybridization, effects of substitution, solvent effects.

### **STRUCTURE OF ORGANIC COMPOUNDS**

Isomerism; Structural [chain, position, functional group, metamerism, tautomerism], stereoisomerism. Introduction to conformational analysis of alkanes (Ethane and butane) and cycloalkanes (cyclohexane). Geometrical isomerism (Cis and Trans configuration in alkene and cycloalkane). Optical isomerism with one and two chiral carbons. Racemisation and resolution of racemic mixtures.

### **BOOKS RECOMMENDED**

1. Whitten KW, Davis RE, Peck LM and Stanley G "General Chemistry" 7<sup>th</sup> Ed (2004) Thomas Learning
2. Ralph PH and Harwood WS "General Chemistry: Principles and Modern Applications" 8<sup>th</sup> Ed (2002) Prentice Hall
3. Whitten KW, Davis RE, Peck LM and Stanley G "General Chemistry With Qualitative Analysis" 6<sup>th</sup> Ed (2002) Thomas Learning
4. Manahan SE "Environmental Chemistry" 6<sup>th</sup> Ed (1994) Lewis Publisher
5. Dara SS "Environmental Chemistry and Pollution Control" 1<sup>st</sup> Ed (1993) S Chand & Co. Ltd., Delhi
6. Chang R "Chemistry" 7<sup>th</sup> Ed (2002) McGraw Hill, Higher education Commission
7. Atkins PW and Shriver DF "Inorganic Chemistry" 3<sup>rd</sup> Ed (1999) W. H. Freeman & Co.
8. Seager SL and Slabaugh MR "Chemistry for Today" 4<sup>th</sup> Ed (2000) Thomas Learning
9. Mackay KM, Mackay RA and Henderson W "Introduction to Modern Inorganic Chemistry" (2000) Stanley Thomes Publisher
10. Mc. Murry and Fay "Chemistry" 2<sup>nd</sup> Ed (1998) Prentice-Hall International
11. Petrucci RH "General Chemistry" (1996) Prentice-Hall Inc
12. Segal BG "Experiment and Theory" 2<sup>nd</sup> Ed (1989) John Wiley & Sons
13. Brady JE "General Chemistry: Principles & Structures" (1990) John Wiley & Sons
14. Brady JE and Holum "The Study of Water and its Changes" 2<sup>nd</sup> Ed (1996) John Wiley & Sons
15. Solomons TWG "Organic chemistry" 5<sup>th</sup> Ed (1992) John Wiley & Sons Inc. New York
16. Morrison RT and Boyd RN "Organic Chemistry" 6<sup>th</sup> Ed (1992) Prentice-Hall of India Pvt. Ltd. New Delhi
17. Sykes P "A Guide Book to Mechanism in Organic Chemistry" 6<sup>th</sup> Ed (1996) John Wiley & Sons Inc New York
18. Streitwieser JRA and Heathcock CH "Introduction to Organic Chemistry" 3<sup>rd</sup> Ed (1989) Macmillan Publishing Company, New York

## **CHM-302(Minor) ORGANIC CHEMISTRY**

Credit Hours: (2+1)

### **1. CHEMISTRY OF HYDROCARBONS**

#### **A) ALKANES**

Nomenclature, natural occurrence and physical properties

Preparation of alkanes: Hydrogenation of alkenes; Reduction of alkyl halides [Hydrolysis of grignard reagent and reduction by metal and acid; Reduction by alkali metal hydrides Wurtz reaction; Kolb's electrolysis.

Reactions of alkanes: Oxidation of alkanes; Combustion, energy of activation and heat of reaction; Halogenation of alkanes; Mechanism of halogenation; Orientation of halogenation Free radical reactions, stability of free radicals, orientation and reactivity of free radicals, stability and reactivity of free radicals. Sulfochlorination, Intermediates for the production of detergents; Nitration; Insertion of methylene group; Pyrolysis: Cracking.

#### **B) ALKENES**

Nomenclature, natural occurrence and physical properties Preparations of alkenes: Partial hydrogenation of alkynes; Dehydration of alcohols [Pyrolytic dehydration, acid catalysed dehydration]; Dehydrohalogenation of alkyl halides; Dehalogenation of vicinal dihalides. Reactions of Alkenes: Electrophilic addition reactions [Addition of hydrogen halides, halogens, sulfuric acid, water (hydration), hypohalous acid]. Mechanism of electrophilic addition reactions and orientation of addition (Markonikov's rule). Formation and relative stability of carbonium ions. Radical addition to alkenes [Anti-markonikov addition of hydrogen bromide. Oxidation of alkenes; Oxidative cleavage of alkenes.; Hydroxylation with OsO<sub>4</sub> and KMnO<sub>4</sub>; Degradation by ozonolysis; Epoxidation by peroxyacids.

#### **C) ALKYNES**

Nomenclature, natural occurrence and physical properties; Preparation of alkynes: Dehydrohalogenation of alkyl dihalides; Reactions of Alkynes: Addition reactions (addition of halogens and hydrogen halide). Oxidative cleavage of alkynes

#### **D) CYCLOALKANES (ALICYCLIC COMPOUNDS)**

Nomenclature, natural occurrence and physical properties; Relative stability of small, normal, medium and large sized rings; Synthesis of three, four, five and six membered rings. Reactions of cycloalkanes; Ring opening reactions. Ring expansion reactions.

#### **2. AROMATIC HYDROCARBONS AND HETEROCYCLIC COMPOUNDS**

Nomenclature of simple aromatic systems and five and six membered heterocyclic rings containing O, N and S. Aromaticity. Preparation of aromatic compounds. Synthesis of benzene, pyridine and furane. Preparation of condensed aromatic systems (naphthalene and anthracene). Reactions of aromatic compounds.

Comparison of reactivity of benzene, aromatic heterocyclic systems and condensed aromatic systems. Electrophilic substitution reactions of benzene and heterocyclic aromatic compounds (five and six membered) including nitration, sulfonation, halogenation, Friedel-Crafts acylation and Friedel-Crafts alkylation. Mechanism of electrophilic substitution reactions. Orientation in benzene. Oxidation of alkyl benzene.

#### **3. ALKYL HALIDES**

Nomenclature, classification and physical properties; Preparation of alkyl halides: From alcohols; Halogenation of certain hydrocarbons; Addition of HX and X<sub>2</sub> to alkenes and alkynes; Hunsdiecker reaction; Haloform reaction. Reactions of alkyl halides: Nucleophilic substitution reactions; Mechanism of Nucleophilic substitution reactions. Elimination reactions; (Zaitsev rule and Hofmann rule). Competition between S<sub>N</sub> and elimination reactions; Grignard reagent: Preparation and reactions.

#### **4. CHEMISTRY OF HYDROXYL GROUP AND ETHERS**

Nomenclature, classification and physical properties of alcohols, phenols and ethers; Preparation of alcohols: Hydroboration-oxidation of alkenes. Reaction of Grignard reagent with carbonyl compounds. Hydrolysis of alkyl halides Reduction of carbonyl compounds, acids and esters. Hydroxylation of alkenes. Reactions of Alcohols: Acid catalyzed reaction of alcohols with HX. Oxidation of alcohols. Preparation of phenols: Hydrolysis of diazonium salts Alkali fusion of sulfonates. Hydrolysis of aryl halides. Reactions of phenols : Acidity

(salt formation). Ester formation. Electrophilic substitution reaction (Halogenation, nitration, sulfonation, Friedel-Crafts alkylation and Friedel-Crafts acylation, nitrosation). Ether formation (Williamson's synthesis). Preparation of ethers: Reactions of ethers; Cleavage by acids.

## **5. CHEMISTRY OF CARBONYL COMPOUNDS**

Comparative study of Structure and reactivity of aldehydes, ketones, carboxylic acids and their derivatives.

### **A) ALDEHYDES AND KETONES**

Nomenclature, natural occurrence and physical properties. Preparation of aldehydes and ketones; Oxidation of 1° and 2° alcohols; Friedel-Crafts acylation (for aromatic carbonyl compounds); Hydration of alkynes; Glycol cleavage; Ozonolysis of alkenes. Reactions of aldehydes and ketones; Nucleophilic Addition Reactions; Hydration and Hemiacetal Formation; Acetal Formation; Formation of Imines and Related Compounds; Enamine Formation; Cyanohydrin Formation; Reduction by Complex Metal Hydrides; Addition of Organometallic Reagents; Reactions at the  $\alpha$ -Carbon; The Aldol Reaction; Dehydration of Aldol Products; Mixed Aldol Condensations. Other Carbonyl Group Reactions; Reduction (Wolff-Kishner Reduction, Clemmensen Reduction and Hydrogenolysis of Thioacetals); Oxidation (Tollens test, Benedict's test and Fehling's test).; Cannizzarro's reaction; Halogenation of ketones.

### **B) CARBOXYLIC ACIDS AND THEIR DERIVATIVES**

Nomenclature, natural occurrence and physical properties. Preparation of carboxylic acids; Oxidation of primary alcohols; Oxidation of alkylbenzenes; Carbonation of grignard reagent; Hydrolysis of nitriles. Reactions of carboxylic acids: Acidity: Salt formation; Conversion into functional derivatives. Conversion into acid chlorides Conversion into anhydrides. Conversion into esters. Conversion into amides.

## **6. CHEMISTRY OF AMINES**

Nomenclature, classification and physical properties of amines. Preparation and reactions of amines.

## **7. CARBOHYDRATES**

Introduction. Classification Mono, di- and polysaccharides; Aldoses and hexoses; Reducing and non-reducing sugars. Structure: Cyclic forms of monosaccharides; The configuration and important reactions of glucose.

## *PRACTICALS*

### **QUALITATIVE ORGANIC ANALYSIS**

Identification of compound containing C, H, O and N or S and functional groups [Hydrocarbon, Carboxylic acid, Phenol, Amide, thioamide, Aldehyde or Kketone]. Preparation of their derivatives. Quantitative analysis of organic compounds containing COOH group. Synthesis of organic compounds: phthalimide and iodoform. Isolation of compounds from natural products: casein from milk and isolation of starch from potato.

### **BOOKS RECOMMENDED**

1. Solomons TWG "Organic chemistry" 5<sup>th</sup> Ed (1992) John Wiley & Sons Inc. New York
2. Morrison RT and Boyd RN "Organic Chemistry" 6<sup>th</sup> Ed (1992) Prentice-Hall of India Pvt. Ltd. New Delhi
3. Sykes P "A Guide Book to Mechanism in Organic Chemistry" 6<sup>th</sup> Ed (1986) John Wiley & Sons Inc. New York
4. Streitwieser JRA and Heathcock CH "Introduction to Organic Chemistry" 3<sup>rd</sup> Ed (1989) Macmillan Publishing Company, New York
5. Furniss BS, Hannaford AJ, Smith PWG and Tatchell AR "Vogel's Textbook of Practical Organic Chemistry" 5<sup>th</sup> Ed (2000) Longman Scientific & Technical, UK
6. Arayne MS & Sultana "A Manual of Qualitative Organic Analysis" 3<sup>rd</sup> Ed (2006) BCCT University of Karachi

## SEMESTER-II

### **CHM-312 ORGANIC CHEMISTRY**

Credit Hours: (2+1)

#### **BASIC CONCEPTS OF ORGANIC CHEMISTRY**

Bonding in organic compounds; Relation of structure with physical properties; Reactivity of organic compounds. Oxidation states of carbon; Structure and stability of reactive intermediates (carbocations, carbanions, free radicals and carbenes). Electrophiles and Nucleophiles. The arrow notation in reaction mechanism. Types of reactions: Substitution reactions. Elimination reactions. Addition reactions. Factors effecting reactions (reaction mechanism): Electronic effects (Resonance and Mesomeric effects). Steric effects. Solvent effects. Structural effects (point b).

#### **ISOMERISM**

Structural isomerism [chain, position, functional group, metamerism, tautomerism] Stereoisomerism; Introduction to conformational analysis of alkanes (Ethane and butane) and cycloalkanes (cyclohexane); Geometrical isomerism (Cis and Trans configuration in alkenes and cycloalkanes); Optical isomerism with one and two chiral carbons. Racemisation and resolution of racemic mixtures.

#### **CHEMISTRY OF ALKANES AND CYCLOALKANES**

Electronic effects; steric effects; effects of hybridization; effects of substitution; solvent effects: ALKANES: Nomenclature, Natural occurrence and Physical properties Preparation of alkanes: Hydrogenation of alkenes Reduction of alkyl halides [Hydrolysis of grignard reagent and reduction by metal and acid Reduction by alkali metal hydrides; Wurtz reaction; Kolb's electrolysis. Reactions of alkanes: Oxidation of alkanes; Combustion, energy of activation and heat of reaction; Halogenation of alkanes; Mechanism of halogenation; Orientation of halogenation ; Free radical reactions, stability of free radicals, orientation and reactivity of free radicals, stability and

reactivity of free radicals;.Sulfochlorination; Intermediates for the production of detergents; Nitration; Insertion of methylene group; Pyrolysis: Cracking.

### **CYCLOALKANES (ALICYCLIC COMPOUNDS)**

Nomenclature, natural occurrence and physical properties; Relative stability of small, normal, medium and large sized rings. Synthesis of three, four, five and six membered rings. Reactions of cycloalkanes ; Ring opening reactions.Ring expansion reactions.

### **CHEMISTRY OF ALKENES AND ALKYNE ALKENES**

Nomenclature, natural occurrence, physical properties and acidity of alkynes. Preparations of alkenes: Partial hydrogenation of alkynes; Dehydration of alcohols[Pyrolytic dehydration, acid catalysed dehydration]; Dehydrohalogenation of alkyl halides; Dehalogenation of vicinal dihalides. Reactions of alkenes: Electrophilic addition reactions [Addition of hydrogen halides, halogens, sulfuric acid, water (hydration) and hypohalous acid]. Mechanism of electrophilic addition reactions and orientation of addition (Markonikov's rule). Formation and relative stability of carbonium ions. Radical addition to alkenes [Anti-markonikov addition of hydrogen bromide. Oxidation of alkenes Oxidative cleavage of alkenes. Hydroxylation with  $\text{OsO}_4$  and  $\text{KMnO}_4$ . Degradation by ozonolysis. Epoxidation by peroxyacids. Reactions of conjugated dienes: Preparation of alkynes: Dehydrohalogenation of alkyl dihalides; Reactions of Alkynes: Addition reactions (addition of halogens and hydrogen halide). Substitution reactions of alkynes. Oxidative cleavage of alkynes.

### **AROMATIC HYDROCARBONS AND HETEROCYCLIC COMPOUNDS**

Nomenclature of simple aromatic systems and five and six membered heterocyclic rings containing O, N and S. Aromaticity. Preparation of aromatic compounds; Synthesis of benzene, pyridine and furane. Preparation of condensed aromatic systems (naphthalene and anthracene). Reactions of aromatic compounds; Comparison of reactivity of benzene, aromatic heterocyclic systems and condensed aromatic systems. Electrophilic substitution reactions of benzene, heterocyclic aromatic compounds (5 and 6 membered) and condensed aromatic systems (naphthalene and anthracene) including nitration,

sulfonation, halogenation, Friedel-Crafts acylation and Friedel-Crafts alkylation. Mechanism of Electrophilic substitution reactions. Orientation in benzene. Reaction of alkyl benzene side chain vs. ring. Oxidation of alkyl benzene.

#### **7. ALKYL HALIDES**

Nomenclature, classification and physical properties; Preparation of alkyl halides: From alcohols; Halogenation of certain hydrocarbons; Addition of HX and X<sub>2</sub> to alkenes and alkynes; Hunsdiecker reaction; Haloform reaction. Reactions of alkyl halides: Nucleophilic substitution reactions; Mechanism of Nucleophilic substitution reactions; Elimination reactions; Mechanism of Elimination reactions; Orientation of Elimination reactions (Zaitsev rule and Hofmann rule. Competition between SN and elimination reactions. Grignard reagent: Preparation and reactions.

#### **PRACTICAL**

##### **QUALITATIVE ORGANIC ANALYSIS**

Identification of compounds containing C, H, O and N or S and functional groups [Hydrocarbons, Carboxylic acids, Phenols, Amides, Thioamides, Aldehydes or ketones]. Preparation of their derivatives.

##### **ISOLATION OF COMPOUNDS FROM NATURAL PRODUCTS**

Introduction of Natural Product (dry lab) ; Isolation of casein from milk; Isolation of Starch from potato; Paper chromatography of pigments (spinach).

##### **BOOKS RECOMMENDED**

1. Solomons TWG "Organic chemistry" 5<sup>th</sup> Ed (1992) John Wiley & Sons Inc. New York
2. Morrison RT and Boyd RN "Organic Chemistry" 6<sup>th</sup> Ed (1992) Prentice-Hall of India Pvt. Ltd. New Delhi
3. Sykes P "A Guide Book to Mechanism in Organic Chemistry" 6<sup>th</sup> Ed (1986) John Wiley & Sons Inc. New York
4. Streitwieser JRA and Heathcock CH "Introduction to Organic Chemistry" 3<sup>rd</sup> Ed (1989) Macmillan Publishing Company, New York

5. Furniss BS, Hannaford AJ, Smith PWG and Tatchell AR "Vogel's Textbook of Practical Organic Chemistry" 5<sup>th</sup> Ed (1989) Longman Scientific & Technical, UK

## **BS CHEMISTRY SECOND YEAR**

### SEMESTER-III

#### **CHM-411 PHYSICAL CHEMISTRY**

Credit Hours: (2+1)

#### **ELECTROCHEMISTRY**

Introduction to electrochemical processes: Redox Reactions, electrode potential of a cell. Nernst theory of electrode potential. Quantitative aspects of electrolysis. Electrolysis of molten salts. Electrolysis of aqueous solutions. Laws of electrolysis. Characteristics of working cell. Corrosion, rate of corrosion, inhibition of corrosion.

The electrical currents in ionic solutions: Conductivities and their measurements. Migration of ions, ionic mobilities, measurements of ionic mobilities. Molar conductance of electrolytes at infinite dilution. Transference numbers and their determination. Influence of various factors on conductance. Applications of conductance measurement.

#### **SOLUTION**

The properties of simple mixtures/ solutions. Concentration terms. The thermodynamic description of mixtures. Partial molar quantities. The chemical potential of liquids. Ideal solutions. Raoult's law. The properties of solutions: liquid mixtures, colligative properties. The common features of colligative properties, elevation of boiling point, depression of freezing point, solubility, Osmosis and Osmotic pressure, solvent and solute activity. Vant Hoff's theory of dilute solutions. pH and pOH of solutions, Acid/Base ionization constants. Relationship of acidity and basicity with dissociation constant. Buffer solutions,

Composition and action of buffer solution, buffer capacity. Henderson-Hasselbalch relation. pH control in biological systems.

### **THERMODYNAMICS AND THERMOCHEMISTRY**

The basic concepts: systems, properties, state functions, thermodynamic processes, work heat and energy. The first law of thermodynamics. Change in internal energy during reversible and irreversible isothermal and adiabatic expansion and compression. Calorimetry. Heat and Enthalpy: Heat capacity at constant volume and pressure. The temperature dependence of the Enthalpy. The relation between  $C_p$  and  $C_v$ . Work of adiabatic expansion. The second law of thermodynamics. The directions of spontaneous change. The Entropy and entropy change accompanying specific processes. The Efficiency of the thermal process. Zeroth law. Thermochemistry: Standard enthalpy changes. Hess's law. The Born-Haber cycle. The temperature dependence of reaction enthalpies.

### **THE PROPERTIES OF SURFACES**

Properties of liquid surfaces. Sufactants. The experimental study of surface films, physical properties of monolayer, Langmuir- Blodgett film. Adsorption of liquid on surface, physisorption, chemisorption. Adsorption isotherm: The Langmuir isotherm. The BET isotherm. Freundlich isotherm. Colloidal systems: Introduction, properties of colloids. Classification. Preparation of colloids Macromolecules: Natural and synthetic polymers, reactivity of polymers.

### **PRACTICALS**

1. Determination of composition of unknown sample by surface tension method.
2. Determination of composition of unknown sample by Viscosity method.
3. Determination of the Parachor value of methanol, ethanol and  $\text{CH}_2$  group.
4. Determination of Heat of solution by solubility method.
5. Determination of Heat of neutralization of strong acid and strong base.
6. Determination of the concentration of acid/base by conductance measurement.
7. Determination of the solubility product of sparingly soluble salts by conductance measurement.

### **BOOKS RECOMMENDED**

1. Segal BG "Chemistry Expt. & Thery." (1985) Jhon Willy & Sons, Inc
2. Glasstone S "Physical Chemistry" 2<sup>nd</sup> Ed (1960) Macmillan and Co
3. Maron S H and Prutton CF "Principle of Physical Chemistry" 4<sup>th</sup> Ed (1965) Macmillan Co
4. Castellan GW "Physical Chemistry" 3<sup>rd</sup> Ed (1986) Addison Wesley Publishing Co
5. Atkins PW "Physical Chemistry" 7<sup>th</sup> Ed (2003) Oxf. Uni. Press
6. Petrucci RH and Hill JW "G. Chemistry" (1996) Prentice Hall- Inc
7. Liptrot GF, Thompson J J and Walker GR "Modern Physical Chemistry" (1986) Bell and Hyman Ltd
8. Bursten BL "Chemistry The Central Science" (2002) Prentice Hall International, Inc
9. Chang R. "Chemistry" 7<sup>th</sup> Ed (2002) McGraw-Hill Higher Education

### **CHM-412 ORGANIC CHEMISTRY**

Credit Hours: (2+1)

#### **CHEMISTRY OF ALCOHOLS AND PHENOLS**

Classification and nomenclature of alcohols and phenols and their physical properties. Preparation of alcohols; Hydroboration-oxidation of alkenes. Reaction of grignard reagent with carbonyl compounds. Hydrolysis of alkyl halides. Reduction of carbonyl compounds, acids and esters. Hydroxylation of alkenes. Preparation of phenols: Hydrolysis of diazonium salts. Alkali fusion of sulfonates Hydrolysis of aryl halides. iv) Reactions of Alcohols; Acid catalyzed reaction of alcohols with HX. Formation of alkyl sulfonates. Oxidation of alcohols; Reactions of phenols: Acidity (salt formation) Ester formation Electrophilic substitution reactions. Ether formation (Williamson's synthesis).

#### **CHEMISTRY OF ETHERS**

Nomenclature and physical properties Preparation of ethers Williamson's synthesis Alkoxymercuration-demercuration Preparation of Epoxides from halohydrins Peroxidation of carbon-carbon double bond; Orientation in cleavage of epoxides. Reactions of ethers; Cleavage by acids; Reactions of epoxides: Acid catalyzed cleavage

#### **CHEMISTRY OF CARBONYL COMPOUNDS (ALDEHYDES AND KETONES)**

Nomenclature, natural occurrence and physical properties. (iii) Reactions of aldehydes and ketones; Reversible nucleophilic addition

reactions; Hydration and hemiacetal formation; Acetal formation; Formation of imines and related compounds; Enamine formation; Cyanohydrin formation; Irreversible nucleophilic addition reactions; Reduction by complex metal hydrides; Addition of organometallic Reagents; Reactions at the  $\alpha$ -carbon; The aldol reaction; Dehydration of aldol products; Mixed aldol condensations; Other carbonyl group reactions; Reduction (Wolff-Kishner reduction, Clemmensen reduction and hydrogenolysis of thioacetals). Oxidation (Tollens test, Benedict's test and Fehling's test); Cannizzaro's reaction.; Halogenation of ketones.

### **CHEMISTRY OF CARBOXYLIC ACIDS AND THEIR DERIVATIVES**

Nomenclature, natural occurrence and physical properties. Preparation of carboxylic acids; Oxidation of primary alcohols; and of alkylbenzenes; Carbonation of grignard reagent; Hydrolysis of nitriles. Reactions of carboxylic acids; Acidity: Salt formation; Conversion into acid chlorides; Conversion of carboxylic acids into various functional derivative like acid halides, acid chlorides, anhydrides, esters, amides. Reduction reactions of carboxylic acids.

### **CHEMISTRY OF AMINES**

Nomenclature, classification and physical properties of amines Preparation of amines: Reduction of nitro compounds; Reductive amination; Reduction of nitriles Hofmann degradation Reactions of amines: Basicity; Salt formation; Alkylation; Conversion into amides; Reaction with nitrous acid (diazonium salts); Replacement reactions of diazonium salts.

### **PRACTICAL**

#### **QUANTITATIVE ORGANIC ANALYSIS**

Quantitative analysis of organic compounds containing COOH group

#### **2. SYNTHESIS OF SAMPLE ORGANIC COMPOUNDS**

Synthesis of Benzoic acid from toluene; Synthesis of Iodoform; Synthesis of 2,4,6-Tribromoaniline; Synthesis of Nitrobenzene; Synthesis of phenyl azo-naphthol from 2-naphthol; Synthesis of Phthalimide from phthalic acid.

### **BOOKS RECOMMENDED**

1. Solomons TWG "Organic Chemistry" 5<sup>th</sup> Ed (1992) John Wiley & Sons Inc. New York
2. Morrison RT and Boyd RN "Organic Chemistry" 6<sup>th</sup> Ed (1992) Prentice-Hall of India Pvt. Ltd. New Delhi
3. Sykes P "A Guide Book to Mechanism in Organic Chemistry" 6<sup>th</sup> Ed (1986) John Wiley & Sons Inc. New York
4. Streitwieser JRA and Heathcock CH "Introduction to Organic Chemistry" 3<sup>rd</sup> Ed (1989) Macmillan Publishing Company, New York
5. Finar IL "Organic Chemistry" Vol. I and II, 5<sup>th</sup> Ed (1977) English Language Book Society & Longman group Ltd. London
6. Furniss BS, Hannaford AJ, Smith PWG and Tatchell AR "Vogel's Textbook of Practical Organic Chemistry" 5<sup>th</sup> Ed (1989) Longman Scientific & Technical, UK

### **SEMESTER-III/IV**

#### **CHM-401(Minor) PHYSICAL CHEMISTRY**

Credit Hours: (2+1)

#### **ELECTROCHEMISTRY**

Electrolytic cells, Galvanic and fuel cells, process of electrolysis, electrode process, Ohm's law and electrical units, Faraday laws of electrolysis, coulometry, Conductance measurement and its applications. Theory of redox reaction, Nernst equation and its applications. Types of electrodes (reference and test), Electrochemical techniques including pH-metry, potentiometry, and coulometry, related numericals. Corrosion and methods of preventing corrosion.

#### **CHEMICAL KINETICS**

Introduction to chemical kinetics. Use of kinetics to fundamental and applied sciences, time scales of chemical reactions. Reaction rates and rate laws and their relation to stoichiometry. Order of reaction and molecularity, First and second order reactions. Various methods (differential, integral, and half life) to determine order of reaction. Arrhenius equation for the temperature dependence of the rate of simple reactions. Basic collision theory and transition state theory for reaction rate, activation energy. Catalysis, principle of catalyst, heterogeneous and homogeneous catalysis and their industrial applications. Reaction mechanism. Chain reactions.

#### **CHEMICAL EQUILIBRIUM**

Dynamic and static equilibrium., factors effecting equilibrium. Homogeneous and heterogeneous equilibrium with examples. Law of mass action, Le chatelier's principle and its impact on equilibrium position. Calculation of equilibrium constant. Relation between  $K_c$ ,  $K_p$  with examples. Solubility and solubility product. Common ion effect. Distribution law. Application of distribution law and its validity (solvent extraction, determination of  $K_{eqb}$ . for  $I_2$  &  $I_3^-$ , system, chromatography).

### **THERMODYNAMICS AND THERMOCHEMISTRY**

Zeroth, first, and second laws of thermodynamics, state functions, system and its surrounding, thermodynamic reversibility and irreversibility. Work done and the change of internal energy during isothermal expansion of an ideal gas. Change of internal energy due to heat transfer at constant volume and constant pressure. Heat capacities of a gas at constant volume and constant pressure. Thermochemistry, enthalpy, entropy. Standard states. Hess's Law.

### **SURFACE PHENOMENA AND COLLOIDS**

Adsorption and types of adsorption. Langmuir and Freundlich adsorption isotherm. Application of adsorption. Colloids, types of colloids, properties and preparation of colloidal solution. Examples of surface phenomena.

### **PRACTICALS**

- i) Determination of percentage composition of unknown sample by viscosity method.
- ii) Determination of percentage composition of unknown sample by surface tension method.
- ii) Determination of Parachor value by surface tension method
- iii) Determination of heat of solution by solubility method
- iv) Determination of solubility and solubility product of a sparingly soluble salts
- v) To study the kinetics of first order reaction
- vi) To study the kinetics of second order reaction
- vii) To construct Freundlich Adsorption isotherm of acetic acid on charcoal.

### **BOOKS RECOMMENDED**

1. Atkins PW "Physical Chemistry" 7<sup>th</sup> Ed (2003) Oxford University Press

2. Atkins PW "Elements of Physical Chemistry" 3<sup>rd</sup> Ed (2003) Oxford University Press
3. Liprot GF "Modern Physical Chemistry" (1982) ELBS
4. Holum B "Fundamentals of Chemistry" 3<sup>rd</sup> Ed (1988) John Wiley Inc
5. Silberbery "Chemistry: The Molecular Nature of Matter and Change" 2<sup>nd</sup> Ed (2000) Mc Graw Hill
6. Matthews P "Advanced Chemistry" Vol I and II (1992) Cambridge University Press
7. Johnson BR and Scott SK "Beginning Calculations in Physical Chemistry" (1997) Oxford
8. Berry RS, Rice SA and Ross J "Physical Chemistry" (1980) John Wiley & Sons

### **CHM-402(MINOR) INORGANIC CHEMISTRY**

Credit Hours: (2+1)

#### **ACIDS AND BASES**

Review of the concepts of Chemical Equilibrium, Arrhenius and Bronsted- theories of acids and bases, Self-Ionization of water, pH scale,  $K_w$ , Strong and Weak Acids and Bases,  $K_a$  and  $K_b$ , Polyprotic Acids, Ions as Acids and Bases, Common Ion Effect in acid base Equilibria, Buffer Solutions, Molecular structure and acid base behaviour. Indicators, Neutralization Reactions, Titration Curves, Solutions of Salts of Polyprotic Acids, Solubility Equilibria, pH, Lewis Acids and Bases, Hard and Soft Acids and Bases.

#### **THEORIES OF BONDING**

Interatomic bond and Intermolecular bond. Nature of covalent bond in terms of Valence Bond Theory, Molecular structure, Molecular orbital Theory (Diatomic Molecules).

#### **CHEMISTRY OF S-BLOCK ELEMENTS**

Group Trends, General characteristics, Important compounds of s-block elements.

#### **COORDINATION CHEMISTRY**

Introduction, application of complex compounds, Ligands and their types, Nomenclature, The concept of Effective Atomic Number, Coordination Number, Geometry of Complex Ions, Isomerism in complexes, Bonding in complex Ions : Applications of Valence Bond

theory (Linear, Trigonal Planar, Square Planar, Tetrahedral, Square Pyramidal, Trigonal Bipyramidal, Octahedral), Crystal Field theory (Octahedral and Tetrahedral Complexes).

### **PRACTICALS**

Volumetric analysis of various cations and anions. Gravimetric analysis of various cations and anions. Reactions of complex cations. pH Titrations. Equilibrium constant of complexes

### **BOOKS RECOMMENDED**

1. Whitten KW, Raymond ED, Larry MP and Stanely G "General Chemistry" 7<sup>th</sup> Ed (2004) Thomas Learning
2. Hill JW and Petrucci RH "General Chemistry" 8<sup>th</sup> Ed (2002) Printice Hall
3. Masterton WL "Chemistry: Principles and Reactions" (2000) John Wiley and Sons, Inc
4. Zlewsky AV "Stereochemistry of Coordination compounds" (1996) John Wiley & Sons, Inc
5. Harwood WS and Petrucci RH "General Chemistry" (1993) Macmillan Publishing Company
6. Sharpe AG "Inorganic Chemistry" (1992) Longman
7. Shriver DF, Atkins PW and Langford CH "Inorganic Chemistry" (1990) Oxford
8. Brady JE, Russel JW and Holum JR "Chemistry Matter and its Changes" (1989) Saunders College Publishing
9. Vogel AI "Textbook of Quantitative Inorganic Analysis" (1989) Longman Group, Printed in Great Britain by Bath Press Ltd
10. Cotton A and Wilkinson G "Basic Inorganic Chemistry" (1987) John Wiley & Sons
11. Basolo F and Johnson "Coordination Chemistry" (1964) W. A. Benjamin Inc

## SEMESTER-IV

### CHM-421 PHYSICAL CHEMISTRY

Credit Hours: (2+1)

#### CHEMICAL EQUILIBRIUM

Spontaneous chemical reactions and equilibrium. Properties of equilibrium state. Effects of external stress on equilibria (Le Chatelier's Principle), the reaction quotient, Response of equilibria to the conditions such as concentration, pressure, temperature. Relationship between  $K_c$  and  $K_p$ . Heterogeneous equilibria. The nature of solubility equilibria. Distribution law and its validity. Application of the distribution law to the selected systems like solvent extraction, extraction of metals from their ore, investigation of complex ions, chromatography, acid base equilibrium and biological activity.

#### INTRODUCTION TO PHASE EQUILIBRIA

Phase, component and degree of freedom. Phase rule and its applications. One component system (water, carbon dioxide). Polymorphism, enantiotropy. Two component systems (sulphur, Pb, Ag system). Vapour pressure diagram. Temperature composition diagrams. Azeotropes. Liquid-liquid phase. Liquid-solid phase.

### CHEMICAL KINETICS/KINETICS IN LIQUID PHASE

Introduction and Scope of Chemical Kinetics. Experimental techniques for the determination of reaction rate, real time analysis, quenching method, flow method, stopped flow technique, flash photolysis, electrochemical analysis. Factors affecting the rate of chemical reaction. Order and molecularity. Kinetics of Zero order reaction, first order reaction, second reaction order (with same initial concentration), pseudo order reactions. Half life for various order reactions. Methods for the determination of order of reactions. The collision Theory. The Transition State Theory. The Arrhenius Theory. Activation parameters. The kinetics and mechanism of complex reactions: chain reaction, polymerization, catalysis and oscillation.

### CHEMICAL DYNAMICS IN GASES

The Postulates of kinetic theory of Gases. Translational K.E. of molecules, kinetic theory of temperature. Energy units for PV and RT. Mean Square velocity & Root mean square velocity, Graham's law of effusion. Distribution of molecular velocities, Vander Waal's equation.

### PRACTICALS

1. Iodometric titration of sodium thiosulphate with potm. dichromate.
2. Determination of the partition co-efficient of iodine in  $\text{CCl}_4$
3. To determine the equilibrium constant for the reaction  $\text{I}_2$  &  $\text{I}_3^-$  syst.
4. Determination of the equilibrium constant of esterification reaction.
5. To study the kinetics of 1st order reaction.
6. To determine the second order rate constant and calculate half life of the reaction.

### BOOKS RECOMMENDED

1. Segal BG "Chemistry Experiment and Theory " (1985) John Willy & Sons, Inc
2. Castellan GW "Physical Chemistry" 3<sup>rd</sup> Ed (1986) Addison Wesley Publishing Co
3. Atkins PW "Physical Chemistry" 7<sup>th</sup> Ed (2003) Oxford Uni. Press
4. Glasstone S "Thermodynamics for Chemists" 11<sup>th</sup> Ed (1964) East West Press Ltd
5. Petrucci RH and Hill JW "General Chemistry" (1996) Prentice Hall- Inc

6. Liptrot GF, Thompson JJ and Walker GR "Modern Physical Chemistry" (1986) Bell and Hyman Ltd
7. Bursten BL "Chemistry The Central Science" (2002) Prentice Hall International, Inc
8. Chang R "Chemistry" 7<sup>th</sup> Ed (2002) McGraw-Hill Higher Education
9. Liptrot GF "Modern Physical Chemistry" (1982) ELBS. Bell and Hyman Ltd

### **CHM-422 INORGANIC CHEMISTRY**

Credit Hours: (2+1)

#### **ACIDS AND BASES**

Review of the concepts of Chemical Equilibrium, Arrhenius and Bronsted theories of acids and bases, Self-Ionization of water, pH scale,  $K_w$ , Strong and Weak Acids and Bases,  $K_a$  and  $K_b$ , Polyprotic Acids, Ions as Acids and Bases, Common Ion Effect in acid base Equilibria, Buffer Solutions, Molecular structure and acid base behaviour. Indicators, Neutralization Reactions, Titration Curves, Solutions of Salts of Polyprotic Acids, Solubility Equilibria, pH, Lewis Acids and Bases, Hard and Soft Acids and Bases.

#### **THEORIES OF BONDING**

Interatomic bond and Intermolecular bond. Nature of covalent bond in terms of Valence Bond Theory, Molecular structure, Molecular orbital Theory (Diatomic Molecules).

#### **CHEMISTRY OF s-BLOCK ELEMENTS**

Group Trends, General characteristics, Important compounds of s-block elements.

#### **COORDINATION CHEMISTRY**

Introduction, application of complex compounds, Ligands and their types, Nomenclature, The concept of Effective Atomic Number, Coordination Number, Geometry of Complex Ions, Isomerism in complexes, Bonding in complex Ions : Applications of Valence Bond theory (Linear, Trigonal Planar, Square Planar, Tetrahedral, Square Pyramidal, Trigonal Bipyramidal, Octahedral), Crystal Field theory (Octahedral and Tetrahedral Complexes).

#### **PRACTICALS**

Volumetric analysis of various cations and anions. Gravimetric analysis of various cations and anions. Reactions of complex cations. pH Titrations. Equilibrium constant of complexes

#### **BOOKS RECOMMENDED**

1. Whitten KW, Raymond ED, Larry MP and Stanely G "General Chemistry" 7<sup>th</sup> Ed (2004) Thomas Learning
2. Hill JW and Petrucci RH "General Chemistry" 8<sup>th</sup> Ed (2002) Printice Hall
3. Masterton WL "Chemistry: Principles and Reactions" (2000) John Wiley and Sons, Inc
4. Zlewsky AV "Stereochemistry of Coordination compounds" (1996) John Wiley & Sons, Inc
5. Harwood WS and Petrucci RH "General Chemistry" (1993) Macmillan Publishing Company
6. Sharpe AG "Inorganic Chemistry" (1992) Longman
7. Shriver DF, Atkins PW and Langford CH "Inorg Chem" (1990) Oxf
8. Brady JE, Russel JW and Holum JR "Chemistry Matter and its Changes" (1989) Saunders College Publishing
9. Vogel AI "Textbook of Quantitative Inorganic Analysis" (1989) Longman Group, Printed in Great Britain by Bath Press Ltd
10. Basolo F and Johnson "Coordination Chemistry" (1964) W. A. Benjamin Inc

### **BS CHEMISTRY THIRD YEAR SEMESTER-V**

#### **CHM-511 ANALYTICAL CHEMISTRY**

Credit Hours: (2+1)

#### **INTRODUCTION**

An introduction to analytical chemistry. Scope of analytical chemistry, major steps in total chemical analysis, and a general survey of all analytical methods.

#### **ERRORS IN CHEMICAL ANALYSIS**

Evaluation of reliability of analytical data, significant figures, selection of central best value from a set of data, precision and accuracy, methods to measure precision, classification of errors, the distribution of data from replicate measurements, comparison of results Student 't' test. Modern trends in quality control.

## **ATOMIC SPECTROSCOPY**

An introduction to the instrumentation of AAS. Atomic absorption spectroscopy, atomic emission spectroscopy, flame emission spectroscopy, a basic introduction to inductively coupled plasma (ICP) and atomic fluorescence.

## **MOLECULAR SPECTROSCOPY**

Electromagnetic radiation, wave and particle concept, scattering, reflection, refraction and dispersion of light by matter, line and band spectrum molecules. The phenomenon of fluorescence and phosphorescence, absorption laws deviations from the Beer's law, chemical reactions and refractive index.

## **OPTICAL METHODS OF ANALYSIS**

a) Main components of a spectrophotometer, difference between a colorimeter and a spectrophotometer, UV-visible single beam and double beam spectrophotometer. Selection of wavelength for quantitative analysis, calibration curve and application of Beer's law in quantitative analysis, application of absorbance measurement to locate the end point of titration, simultaneous determination of two components system, determination of the formula of the complex using the absorbance measurements mole ratio method, method of continuous variation, slope ratio method, applications of spectrophotometric data for studying chemical equilibrium and the evaluation of equilibrium constants.

## **ANALYSIS OF REAL SAMPLES**

Sampling, digestion of samples by dry and wet ashing with special reference to Kjeldahl's method for nitrogen determination, fluxes, series dilution for instrumental analysis, standard addition method, internal standard method and numerical problems.

## **CHROMATOGRAPHY**

Introduction, classification and applications of chromatography, theory of chromatography, adsorption chromatography, partition chromatography, efficiency of column, resolution of column, quantitative and qualitative analysis by chromatography. Brief introduction to ion-exchange chromatography, gas liquid chromatography, and high pressure liquid chromatography.

## **PRACTICALS**

Separation of ink components by paper chromatography. Determination of metal ion concentration by ion-exchange chromatography. To determine the (i) Wavelength of maximum absorbance (ii) Study the

effect of wavelength on molar absorptivity  $\Sigma$  (iii) Study the effect of concentration and path length on absorbance and  $\Sigma$  at the  $\lambda_{\max}$  of  $\text{KMnO}_4$  solution. Analysis of  $\text{KMnO}_4$  in a sample by calibration curve and single point calibration method. Spectrophotometric titration of ferrous ammonium sulfate by standardized potassium permanganate solution. Spectrophotometric determination of iron in a vitamin tablet. Spectrophotometric determination of dissociation constant of an acid base indicator (methyl red). Determination of sodium or potassium in seawater by flame photometry using standard addition method.

#### **BOOKS RECOMMENDED**

1. Braun RD "Introduction to Chemical Analysis" (1985) McGraw Hill Book Company, London
2. Peace BF "Basic Instrumental Analysis" (1980) D Van Nostrand Company, New York
3. Skoog DA, West DM and Holler FJ "Fundamentals of Analytical Chemistry" 8<sup>th</sup> Ed (2004) Saunders Philadelphia
4. Pecsoc RL, Shields LD, Cairns T and McWilliams IG "Modern Methods of Chemical Analysis" (1976) John Wiley and Sons, New York
5. Vogel AI "A Textbook of Inorganic Quantitative Analysis" (1987) Longman
6. Willard HH, Merritt LL (Jr.) and Dean JA "Instrumental Methods of Analysis" (1988) Von Nostrand New York

#### **CHM-521 INDUSTRIAL CHEMISTRY**

Credit Hours: (2+1)

#### **UNIT OPERATIONS IN CHEMICAL ENGINEERING**

Basic Laws, material balance, molecular units, gas laws, mechanical laws, energy balance, equilibrium relationship, steady state.

#### **FLOW OF FLUIDS**

Properties of fluid, fluid static's, manometers, mechanism of flow of fluid, Reynolds number, distribution of velocities, Bernoulli's theorem, friction losses, measurement of fluid.

#### **FLOW OF HEAT**

Fourier's law, thermal conductivity, parallel flow of heat, radial flow of heat, temperature gradient in forced convection, surface coefficient, overall coefficient, boiling liquids, temperature variation in parallel flow and current flow, heat transfer by radiation, Stefan and Boltzmann Law.

## **EVAPORATION**

Types of Evaporators, evaporator capacity, multiple effect evaporator, capacity of multiple effect evaporator, multiple effect calculation

## **DISTILLATION**

Vapour liquid equilibria, boiling point diagram, Raoult's law, relative volatility, constant boiling liquid equilibrium diagram, distillation methods, rectifying columns, fractionating column calculations, reflux ratio plate to plate calculations, petroleum distillation, steam distillation.

## **DRYING**

Classification of dryers, atmospheric compartment dryers, vacuum tray dryers, tunnel dryers, rotary dryers, cylinder dryers and separator dryers.

## **SEPARATORS**

Screens, Tyler standard screen, screen analysis, wire screen, screen opening, average particle size, weight percent retained, cumulative percent oversize, cumulative percent undersize.

## **PRACTICALS**

Cement analysis. Handling and use of laboratory equipment. Sample measurement and methods for absolute accuracy. Application of filtration techniques, purification of the precipitates, titration techniques and techniques related to standard solution preparation. Economical use and application in analysis of some very inexpensive bench chemicals like HCl, Na<sub>2</sub>CO<sub>3</sub>, CaCO<sub>3</sub> and NH<sub>4</sub>HCO<sub>3</sub>. Simple methods for the determination of % purity of some bench chemicals. Calculation of % of CO<sub>3</sub><sup>2-</sup> as an impurity in NaOH. Calculation of % of HCO<sub>3</sub><sup>-</sup> as an impurity in Na<sub>2</sub>CO<sub>3</sub>. Calculation of % of NH<sub>3</sub> in different commercial ammonium salts used in fertilizers.

## **BOOKS RECOMMENDED**

1. Badger WL and Bancharto JT "Introduction to Chemical Engineering" (1960) Mc Graw Hill Koga Kisha. Ltd
2. Buchner W, Schliebs R and Winter G "Industrial Inorganic Chemistry" (1989) KH Buchel

3. Othmer K "Encyclopedia of Chemical Technology" 3<sup>rd</sup> Ed (1982)  
John Wiley & Sons, New York
4. Perry "Chemical Engineering Hand Book" 3<sup>rd</sup> Ed (1950) Mc Graw  
Hill Inc, New York

### **CHM- 531 INORGANIC CHEMISTRY**

Credit Hours: (2+1)

#### **STRUCTURE OF THE ATOM**

- a) Wave properties of the matter, the Schrödinger equation
- b) Applications of wave equation to some simple problem. A particle in one dimension box, a particle in a cubic box, a particle on a ring. Writing Schrödinger equation for simple molecule and ion.

#### **THEORIES OF BONDING**

- a) Valence bond theory, Concept of hybridization, Writing wave equations of hybrid orbitals.
- b) Molecular orbital theory, Writing wave equations of molecules with reference to homonuclear & poly nuclear structure.
- c) Valence Shell Electron Pair Repulsion Theory.

#### **MOLECULAR STRUCTURE**

Prediction of hybridization, geometry and drawing structure of molecules and ions.

#### **4. CHEMISTRY OF NON METALS**

- a) Hydrogen and Hydrides.
- b) Chemistry of noble gases with reference to synthesis properties of Xenon compounds and properties of Xenon compounds. Determination of structure of these compounds.

##### **b) CHEMISTRY OF HALOGENS**

Group trends, preparation and properties of oxides, oxo acids, oxo salts of halogens. Inter halogen and poly halides. Pseudo halogens.

##### **a) CHEMISTRY OF OXYGEN AND SULFUR**

Group trend, Preparation and properties of Oxides, Sulphides and oxoacids of Sulphur

##### **b) CHEMISTRY OF CARBON AND SILICON**

Group trend, Fullerene, Silicones and Silicates

##### **c) CHEMISTRY OF BORON**

General Characteristics of Boron. Preparation, Properties and Structure of Boron Hydride using STYX method. Note: The structure of other nonmetal compounds are covered under molecular structure

### **INORGANIC ENERGETICS**

a) Thermochemistry: System and surroundings, Enthalpy, Thermochemical equations, Law of Thermochemistry, Problem related to calculation of  $\Delta H_{\text{rxn}}$

b) Thermodynamics: Entropy, Free Energy, Relation among  $\Delta G$ ,  $\Delta H$ ,  $\Delta S$  and equilibrium constant  $K$  of a reaction. Problem related to  $\Delta G = \Delta H - T\Delta S$ ,  $\Delta G = -RT \ln K$  and  $\Delta G = -nFE^0$

### **PRACTICALS**

Mixture analysis with three acidic & three basic radicals. Volumetric analysis. Volumetric analysis. Determination of equilibria, Analysis of a mixture of acids, Analysis of a mixture of metals, with complexometry and gravimetry.

### **BOOKS RECOMMENDED**

1. Sharp AG "Inorganic Chemistry" 2<sup>nd</sup> Ed (1986) Addison Wesley Longman Ltd
2. Cotton FA, Wilkinson G, Murillo CA and Bochmann M "Advanced Inorganic Chemistry" 6<sup>th</sup> Ed (1999) John Wiley & Sons, Inc
3. Liptrot GF, Thompson JJ and Walker GR "Modern Inorganic Chemistry" 4<sup>th</sup> Ed (1986) Bell & Hymann Limited
4. Purcell KF and Kotz JC "An Introduction to Inorganic Chemistry" (1980) Saunders College Publishing

### **CHM-541 ORGANIC CHEMISTRY**

Credit Hours: (2+1)

### **HETEROCYCLIC COMPOUNDS**

a) Definition, classification and nomenclature; Heterocyclic compounds containing 2 & 3 hetero-atoms and fused ring system

b) Detailed study of heterocycles including their reaction mechanism furan, nomenclature, molecular orbital picture, resonance hybrids. Preparation of furan and its derivatives: from mucic acid, decomposition of furfural, 1,4-diketo compounds, ethyl acetoacetate, and Fests-Benary Synthesis. Physical properties of furan. Reaction of furan: Addition reactions; hydrogenation, Diels-Alder reaction, 2,5-

addition. Electrophilic substitution reactions: chlorination, nitration, sulfonation, mercuration, Friedel's Craft alkylation and acylation, Gatterman Koch reaction, Gomberg reaction. Formation of organometallic compounds. Formation of pyrrole and thiophene. Ring opening reactions.

c) Pyrrole: nomenclature, molecular orbital picture, resonance hybrids. Preparation of pyrrole and its derivatives: from acetylene, ammonium mucate, succinimide, ethylacetoacetate; Paal Knorr Synthesis, Knorr pyrrole synthesis, Hantzsch synthesis. Physical properties of pyrrole. Reactions of pyrrole: Acidic and Basic character, Resemblance with aromatic amines and phenols. Addition reactions, Electrophilic substitution reactions; chlorination, nitration, sulfonation, Friedel's Craft alkylation and acylation, Gatterman Koch reaction, Reimer Tiemann reaction, Gomberg reaction., ring expansion and reduction.

d) Thiophene: nomenclature, molecular orbital picture, resonance hybrids. Preparation of thiophene and its derivatives; from acetylene, sodium succinate and n-butane. Physical properties of thiophene. Reaction of thiophene: addition reactions, electrophilic substitution reactions; chlorination, bromination, iodination, nitration, mercuration, Friedel's Craft alkylation and acylation, chloromethylation. Formation of organometallic compounds.

e) Pyridine: Molecular orbital picture, resonance hybrids. Preparation of pyridine and its derivatives; from acetylene, Hantzsch synthesis. Physical properties of pyridine. Reactions of pyridine; basic character, reduction, electrophilic substitution reactions; chlorination, nitration. Nucleophilic substitution reaction ; amination, alkylation etc.

### **STEREOCHEMISTRY**

i) Optical activity, Specific rotation, Pasteur's discovery of enantiomers, enantiomers and tetrahedral carbon, chirality, sequence rules for specific rotation.

ii) Diastereomers, Meso compounds, molecules with more than two chiral centers, Racemic mixtures.

iii) Physical properties of stereoisomers, Fisher projections formulas, assigning R and S configurations. Stereoisomerism and chirality in substituted cyclohexanes. E and Z isomerism in alkenes and polyenes.

### **SPECTROSCOPY**

a) Mass Spectrometry; Introduction, Mass spectrometer, mass spectrum, Index of hydrogen deficiency & rule of thirteen, Determination of Molecular weight, Molecular formula from isotope ratio data, Fragmentation patterns; Hydrocarbons, Alcohols and phenols, Aldehydes, Ketones, Esters, Carboxylic acids, Halogen compounds.

b) Infrared Spectroscopy; Introduction, The Infra red absorption process, Use of infra red spectrum, The mode of stretching and bending, Bond properties and absorption trends, The infra red spectrophotometer, Correlation charts and tables.

c) Nuclear magnetic resonance spectroscopy; Introduction, Nuclear spin states, Nuclear magnetic resonance, Absorption energy, The mechanism of absorption (resonance), The chemical shifts and Shielding, The nuclear magnetic resonance spectrometer, Integral and Integration, Chemical environment and chemical shift, Spin-spin splitting ( $n + 1$ ) rule, Pascal's triangle, Coupling constant.

d) Ultraviolet spectroscopy; Introduction, The nature of electronic excitations, The Origin of UV band structure, Principles of absorption spectroscopy, UV spectrophotometer, Presentation of spectra, The effect of conjugation, The Woodward-Fieser Rules for dienes and enones.

e) Combined structural problems-Minimum six solved examples.

## **PRACTICALS**

Separation of 8 – 10 binary mixtures of organic compounds containing various functional groups on the basis of their solubilities and identification of both the components of the mixture.

## **BOOKS RECOMMENDED**

1. Pavia DL, Lampman GM and Kriz G "Introduction to Spectroscopy" 2<sup>nd</sup> Ed (1996) Brace College publishers
2. Whitaker D "Interpreting Organic Spectra" (2000) RSC
3. Clayden J, Greeves N, Warren S and Wothers P "Organic Chemistry" (2001) Oxford University Press
4. Finar IL "Organic Chemistry" Vol I, 6<sup>th</sup> Ed (1973) Longman, London
5. Eliel EI "Stereochemistry of Carbon Compounds" (1975) Mc Graw Hill. Int. Book Co. Singapore
6. Kalsi PS "Stereochemistry conformation and Mechanism" 6<sup>th</sup> Ed (2005) New Age Int. (P) Ltd. Publishers, New Delhi

7. Li JJ "Reactions in Heterocyclic Chemistry" (2005) John. Wiley Int. Singapore
8. Joule J and Smith G " Heterocyclic Chemistry" 2<sup>nd</sup> Ed (1982) Von nostrand Reinhold Compay Ltd, London
9. Joule JA " Heterocyclic Chemistry" (1998) Wiley Int. Singapore

### **CHM-551 PHYSICAL CHEMISTRY**

Credit Hours: (2+1)

#### **ELECTRO CHEMISTRY**

An introduction to electrochemistry, chemical reactions and redox potentials, electrochemical cells, Nernst equation and its application. predicting reactions, stability of oxidation states, cell potential and thermodynamics.

#### **NUCLEAR CHEMISTRY**

Atomic nucleus, nuclides, nuclear stability, modes of decay, nuclear, energetic, nuclear models (shell + liquid drop model), fusion and fission, non spontaneous nuclear processes, nuclear reactors, beta decay systematics, nuclear spins.

#### **RECENT ADVANCES IN ATOMIC STRUCTURE**

Unification theory based upon concepts of quarks, four forces of nature and explanation of quantum numbers proposed and experimentally justified.

#### **KINETIC THEORY OF MATTER**

Theories pertaining to distribution of energies into different groups Maxwell Boltzmann distribution law for energies of molecular systems, method for the determination of Avogadro's number.

#### **PRACTICALS**

To determine the molecular weight of a given polymer by Viscosity method, Titrimetric determination of the effectiveness of an extraction. Determination the concentration of Sodium in a given water sample by Flame Emission Spectrophotometry, To study the Cu-EDTA complex by conductometry method, To study the spectrophotometric titration of Cu (II) with EDTA.

**BOOKS RECOMMENDED**

1. Williams WSC "Nuclear and Particle Physics" (1991) Clarendon Press Oxford
2. Kaplan "Nuclear Physics" (1979) Addison Wesley Publishing Co London
3. Friedlander G, Kennedy JW, Macins S and .Miller JM "Nuclear and `Radiochemistry" 3<sup>rd</sup> Ed (1981) John Wiley and sons New York
4. Vincent "Oxidation and Reduction in Inorganic and Analytical Chemistry" (1985) John Wiley and sons New York
5. Barrow GM "Physical Chemistry" 5<sup>th</sup> Ed (1988) Mc Graw Hill Book Company
6. Jolly WL "Modem Inorganic Chemistry" (1984) Mc Graw Hill Book Company
7. Compton RG and Sanders GHW "Electrode Potentials" (1996) Oxford
8. Winn JS "Physical Chemistry" Harper Collings Publisher 1<sup>st</sup> Ed (1995)

**SEMESTER- VI****CHM-512 ANALYTICAL CHEMISTRY**

Credit Hours: (2+1)

**CONDUCTANCE**

Theory of electrolytes, electrolytic conduction, conductance, specific, equivalent and molar conductance and their dependence on

concentration of strong and weak electrolytes, circuit of conductivity meter, measurements of cell constant, Arrhenius theory of ionization in relation to weak and strong electrolytes, Debye Huckel theory in relation to the ion atmosphere, asymmetry or relaxation effect, solvent effect, electrophoretic effect, Debye Huckel Onsagar equation, ion pair, ion triplet formation, transport numbers of ions, ion motilities and their calculations, types of conduct metric titrations including acid-base titration, precipitation or displacement or replacement titrations, applications of conductance in relation to  $\Lambda_{\alpha}$  &  $K_a$  for weak and strong electrolyte, determination of absolute ionic motilities, solubility of sparingly soluble salts,  $K_w$  (ionic product of water), basicity of an organic acid, speed ratio by transport number, advantages of conduct metric titration over volumetric titration.

### **pH METRY**

Theory of pH metry, self ionization reactions, ionic product of water, acidity and basicity constants, degree of ionization, neutralization reactions, hydrolysis of salt, hydrolytic constants, calculatin of pH/pOH (acids, bases and salt solutions), pH titrations of monoprotic and polyprotic acids, determination of pKa of acids, buffer solutions, buffer capacity and buffer actions, buffer mechanism, preparation and applications of buffers, indicators, theory, indicator constants, preparation an significance of pure and mixed indicators.

### **POTENTIOMETRY**

Theory of potentiometry. Nernt equation. Classification of electrodes, their equations and examples. Reference electrodes (NHE, SCE, Ag/AgCl), test electrodes \*Pt, Glass and ion selective. Standard electrode potential, formal potential, determination ionic strength, activity and activity coefficient. Concentrations cells, liquid junction potential (salt bridge). Types of reactions like neutralization, precipitations, complexations and redox reactions studied by potentiometry, determination of equivalence point by data analysis and other methods.

### **POLAROGRAPHY AND VOLTAMETRY**

Theory of polarography and voltametry. Faradic and non faradic processes. Migration, diffusion and charge currents, polarographic circuits, Fick's diffusion law. Ilkovic and Randles Sevcik equation, supporting electrolytes, potential window, interference from dissolved oxygen, polarographic maxima, type of test electrodes, advantages of mercury test electrode, polarographic techniques like a.c polarographic, pulse polarography, their theory, circuit and advantages, amperometry,

bi- amperometry, their theory, application and advantages, chronopotentiometry, its theory, applications and advantages. Electrogravimetry, types of coulometric titrations, applications, anodic stripping, voltametry, its theory, applications and advantages, numericals based on potentiometry, polarography and coulometry.

### **PRACTICALS**

Calibration of glass wares. Determination of the concentration of acetic acid by potentiometric titration and calculation of the dissociation constant of the acid. The potentiometric titration of diprotic acid with sodium hydroxide, preparation of 1<sup>st</sup> and 2<sup>nd</sup> derivative titration curve. Determination of iron II and iron III in a mixture by potentiometric titration with  $\text{Cr}_2\text{O}_7^{-2}$ . Acid base titration in non aqueous solution

To determine the dissociation constant of weak electrolyte (acetic acid) by conductivity measurement method. To measure the refractive index and dispersive power of various solid and liquid sample. To determine the glucose concentration in the given sample using polarimeter.

### **BOOKS RECOMMENDED**

1. Gross JM and Wiseall B "Principles of Physical Chemistry" (1979) Mc Graw Hill
2. Petrucci RH "General Chemistry" (1996) John Wiley & Ralph, Prentice-Hall Inc
3. Sogal BG "Chemistry: Experiment and Theory" 2<sup>nd</sup> Ed (1989) John Wiley & Sons
4. Vogel AI "Textbook of Quantitative Inorganic Analysis" 5<sup>th</sup> Ed (1994) ELBS UK
5. Harris DC "Quantitative Chemical Analysis" 3<sup>rd</sup> Ed (1991) W.H Freeman & Co., New York USA
6. Atkins PW "Physical Chemistry" 7<sup>th</sup> Ed (2003) Oxford
7. Braun RD "Introduction to Chemical Analysis" Int Ed (1982) Mc Graw Hill
8. Bard J and Faulkner LR "Electrochemical Methods Fundamentals and Application" (1980) John Wiley and Sons, Inc
9. Greef R, Peat R, Peter LM, Pletcher D and Robinson J "Instrumental Method in Electro Chemistry" (1985) John Wiley and Sons New York USA
10. Brett CMA and Brett AMO "Electro Chemistry Principles Methods and Application" (1993) Oxford Science Publication

### **CHM- 522 INDUSTRIAL CHEMISTRY**

Credit hours: (2+1)

## **INTRODUCTION**

Introduction to industrial chemistry and its importance, flow charts, material balance, cost and yield, functions of chemist, chemical process control; In process and finished products control.

## **LEATHER INDUSTRY**

Introduction and uses, Flow sheet of leather, Raw materials, chemicals (pre-tanning, tanning and finishing), Pre- tanning process, Tanning process, Wet Finishing and dry finishing process.

## **DYES**

Introduction, cause of color, chromophores and auxochromes, Classification on the basis of use with one example, mode of absorption and uses of dyes on type of fibers, Dyes intermediates, reactions including nitration , sulphonation, reduction (selection and general), Halogenation on side chain and on the dyes, Sandmayer reaction, carboxylation, alkaline fusion reaction, amination, oxidation, acid dyes, basic dyes, sulfur dyes, vat dyes, reactive dyes, disperse dyes, mordant dyes, azoic dyes, oxidation dyes and non-textile uses of dyes.

## **OILS, FATS AND WAXES**

Introduction, physical properties, types of fatty acids present and uses, Testing methods of fatty acids on GC, Flow sheet diagram of hydrogenated oil, raw oil, degumming, neutralization, bleaching, filtration, hydrogenation, post-neutralization, post bleaching, post filtration, deodorization, chilling, fortification and finished product packing, Production of hydrogen from natural gas cracking unit.

## **SOAPS AND DETERGENTS**

Introduction of soap, Batch Kettle process, flow diagram and details, Monasavon process, Delaval process, sharpless process, introduction to detergent, classification, examples of cationic, anionic, nonionic and amphoteric detergents and their action with water, binders, opacifying agents, flavors, moisturizers of soap industry.

## **GELATIN**

Introduction, uses and types of gelatin, physical and chemical properties of gelatin, Flow sheet diagrams of type A and type B and detailed processing of unit operation.

## **RUBBER INDUSTRY**

Introduction, natural rubber extraction, coagulation, rubber compounding, types of synthetic rubber and synthesis of styrene-butadiene rubber (monomer production and polymer production).

### **SUGAR INDUSTRY**

Introduction, juice extraction, production of raw sugar and cane sugar refining (clarification, filtration, decolorization, recrystallization, centrifugation, drying and conditioning).

### **PESTICIDES**

Introduction, classification of insecticides (chlorinated hydrocarbons, carbamates, organophosphates).classification and examples of herbicides (contact herbicides, systematic herbicides and soil sterilants).rodenticides, fungicides (inorganic and organic fungicides) and germicides.

### **EXPLOSIVES**

Introduction. Classification (primary, secondary and tertiary explosives). Classification based on structural features.

### **PULP AND PAPER INDUSTRY**

Introduction, Types of pulping (mechanical pulping, semi chemical pulping, chemical, solvent pulping and secondary fiber pulping). Bleaching of wood pulp. Manufacture and processing (beating and refining, filling and loading, sizing, sheet forming, pressing and drying).

### **FERMENTATION INDUSTRY**

Introduction. Alcohol fermentation (introduction, uses and process of fermentation). Citric acid production and uses.

### **PHARMACEUTICAL INDUSTRY**

Identification and handling of chemical hazards, consequences of toxic exposures. Validation of pharmaceutical process, Types of validations, documentation, protocol, process flow diagram, process monitoring, sampling and testing, acceptance criteria.

### **PRACTICALS**

1. Determination of concentration of sugar solution by Fehling's solution method.
2. Analysis of vitamins B<sub>12</sub> by spectrophotometric method
3. Determination of percentage purity of amino acid solution by Sorenson formal titration method.

4. Determination of percentage purity of aspirin in the given sample.
5. Determination of percentage of formaldehyde by hydrogen peroxide method.
6. Determination of percentage of formaldehyde by hydrogen peroxide method.
7. Determination of percentage of ascorbic acid in the given sample.
8. Determination of paracetamol content in tablets by spectrophotometric method.
9. Determination of Saponification value of the given oil sample.

#### **BOOKS RECOMMENDED**

1. Kent JA "Riegel's Handbooks of Industrial chemistry" 9<sup>th</sup> Ed (1992) Chapman & Hall
2. Vogel AI "Quantitative Organic Analysis" 5<sup>th</sup> Ed (1994) Longman Group
3. Austin GT "Shreve's Chemical Process Industries" 5<sup>th</sup> Ed (1984) Mc Graw Hill
4. Shreve N "Chemical Process Industries" John Wiley (1982) New York
5. Clark "Isolation and Identification of Drugs and Toxic Substances" (1979)

#### **CHM-532 INORGANIC CHEMISTRY**

Credit Hours: (2+1)

#### **CHEMISTRY OF TRANSITION ELEMENTS**

- a) General characteristics of Transition Metal Elements.
- b) A comparison of First, Second and Third transition series elements.

#### **COORDINATION COMPOUNDS**

##### **I) Crystal field theory:**

Splitting of d-orbitals in an octahedral, tetrahedral, distorted octahedral, square pyramid, square planar and trigonal bipyramid field. Jahn-Teller effect. Calculation of Crystal Field Stabilization. Energies and writing electronic configuration of complex ions. High-spin & Low-spin complexes. Thermodynamic effects of crystal field theory.

##### **II) Molecular Orbital Theory:**

Molecular Orbital Energy diagrams of octahedral, tetrahedral and square planar complexes. Writing molecular orbital configuration of octahedral, tetrahedral and square planar complexes.  $\pi$ -bonding in complexes and its effect on Crystal Field Splitting Energy.

### **MECHANISM OF REACTIONS**

- a) Mechanism of Substitution and Redox reactions.
- b) Trans- Effect.
- c) Synthesis of complex compounds.

### **STABILITY OF COMPLEX IONS**

- a) Factors on which Stability of a Complex ion depends.
- b) Distinction between Thermodynamic and Kinetic Stability.
- c) Stepwise and overall formation Constants of Complex ions.

### **MAGNETIC PROPERTIES OF COMPLEX IONS**

- a) Paramagnetic and diamagnetic complexes.
- b) Calculation of  $\mu_s$ ,  $\mu_{s+L}$ ,  $\mu_{\text{eff}}$  and the relationship between the three.

### **6) ELECTRONIC ABSORPTION SPECTRUM OF TRANSITION METAL COMPLEXES**

- a) Octahedral and tetrahedral complexes.
- b)  $d^2$ - $d^8$  ions Energy level diagram.
- c) Charge transfer spectra.

### **CHEMISTRY OF LANTHANIDE AND ACTINIDE ELEMENTS**

- a) Lanthanides:
  - i) General Characteristics.
  - ii) Lanthanide Contraction.
  - iii) Oxidation States.
  - iv) Occurrence and Isolation.

- b) Actinides:
  - i) General Characteristics.
  - ii) Variable oxidation States.
  - iii) Nuclear Reactions for the synthesis and trans Uranium Elements.

### **PRACTICALS**

Synthesis & characterization of metal complex using substitution & redox reactions.

### **BOOKS RECOMMENDED**

1. Sharpe AG "Inorganic Chemistry" 2<sup>nd</sup> Ed (1986) Addison Wesley Longman Ltd

2. Cotton FA, Wilkinson G, Murillo CA and Bochmann M. "Advanced Inorganic Chemistry" 6<sup>th</sup> Ed (1999) John Wiley and Sons, Inc
3. Huheey JE, Keiter EA and Keiter RL "Inorganic Chemistry" 4<sup>th</sup> Ed (1993) Harper Collins College Publishers
4. Jordan RB "Reaction Mechanism of Inorganic and Organometallic System" (1998) Oxford University Press, Inc
5. Kettle SF "Coordination Compounds" (1969) Thomas Nelson and Sons Ltd

### **CHM-542 ORGANIC CHEMISTRY**

Credit hours: (2 + 1)

#### **NATURAL PRODUCTS**

Introduction to natural product; primary and secondary natural products

#### **ALKALOIDS**

i) Introduction, occurrence, classification, nomenclature.

General methods for the detection of structure of alkaloids; Physical methods: IR, UV, mass, <sup>1</sup>H-NMR and <sup>13</sup>C-NMR spectroscopy and chemical Methods: oxygen functions; hydroxyl, carboxylic, carbonyl, ester, lactone, amido, lactam or betaine, methoxy and methylenedioxy group, Zerwittinoffs active hydrogen, nitrogen functions, determination of basic skeleton: Hoffmann's exhaustive methylation, Emed's modification, Von-Braun's method, ZnCl<sub>2</sub>-distillation, Fusion with KOH, oxidation, reduction; presence of unsaturation.

ii) Coniine; occurrence, isolation, physical properties, medicinal importance. Structural elucidation by chemical methods; structure and molecular formula, ZnCl<sub>2</sub>-distillation, oxidation, reaction with HI, Hoffmann's exhaustive methylation and synthesis of coniine. Structural elucidation by spectroscopic methods; IR, UV, Mass, <sup>1</sup>H-NMR and <sup>13</sup>C-NMR spectroscopy.

iii) Nicotine; occurrence, isolation, physical properties, medicinal importance. Structural elucidation by chemical methods; structure and molecular formula, oxidation, ZnCl<sub>2</sub>-distillation, reaction with HI, reaction with MeI, oxidation of methiodide and synthesis of nicotine. Structural elucidation by spectroscopic methods; IR, UV, Mass, <sup>1</sup>H-NMR and <sup>13</sup>C-NMR spectroscopy.

iv) Papaverine; occurrence, isolation, physical properties, medicinal importance. Structural elucidation by chemical methods: structure and molecular formula, , reaction with HI, reaction with MeI, reaction with

cold  $\text{KMnO}_4$ , reaction with hot  $\text{KMnO}_4$ , reaction with conc.  $\text{KMnO}_4$ ; structural elucidation of veratric, metahemipinic acid, pyridine, 2,3,4-tricarboxylic acid and 6,7-dimethoxy isoquinoline-1-carboxylic acid and synthesis of papaverine. Structural determination by spectroscopic methods; IR, UV, Mass,  $^1\text{H-NMR}$  and  $^{13}\text{C-NMR}$  spectroscopy.

v) Quinine: occurrence, isolation, physical properties, medicinal importance, Structural elucidation by chemical methods; structure and molecular formula, reaction with HI, reaction with MeI, oxidation with  $\text{CrO}_3$ , reaction with bromine, oxidation with acidic  $\text{KMnO}_4$ , oxidation with chromic acid, structure of quinic acid, structure of meroquinine, position of CHO group, and synthesis of quinine. Structural elucidation by spectroscopic methods; IR, UV, Mass,  $^1\text{H-NMR}$  and  $^{13}\text{C-NMR}$  spectroscopy.

### **VITAMINS**

Introduction, Fat soluble vitamins; A, D, E and K. Water soluble vitamins; Vitamin B-complex. Chemistry and structural determination of vitamin  $\text{B}_1$  (Thiamine),  $\text{B}_2$  (Riboflavin) and Vitamin  $\text{B}_6$  (Pyridoxine).

### **CARBOHYDRATES**

Introduction to carbohydrates. Monosaccharides: Aldoses (aldotrioses, aldotetroses, aldopentoses and aldohexoses) and ketoses (trioses, tetroses, pentuloses and hexuloses) and their natural occurrence. Structure of monosaccharides; stereochemistry and absolute configuration, stereochemical relationship with glyceraldehydes. Stereoisomers of aldoses from D and L glyceraldehydes by stepping up with Killiani Fischer synthesis. Ring structure of aldohexoses. Mechanism of mutarotation. Conformations of hexopyranoses and hexofuranoses. The anomeric effect. Determination of ring size of aldoses and pentoses. Structural determination of D-(+)-Glucose: Chemical methods; Chemical reactions to establish presence of an aldehydic group, five hydroxyl groups, linear structure, configuration at 2, 3, 4 and 5 carbon atoms, structural relationship with (+)-mannose and (-)-arabinose and fructose. Spectroscopic methods; IR, Mass and NMR spectroscopy. Reactions of monosaccharides: Reaction with phenyl hydrazine, ether formation (anomeric and other hydroxyl groups) esterification, reduction, oxidation (with  $\text{Br}_2$ ,  $\text{Cu}^{+2}$ ,  $\text{Ag}^{+1}$ ,  $\text{HNO}_3$ ,  $\text{HIO}_4$ ), epimerization, ascending of sugar series (Killiani-Fischer synthesis, Swoden method and wolfrom method), descending sugar series (Wohl method, Ruff's method, Weeman's method), Conversion of an aldose into ketose and ketose into aldose, Lobry de

Bryner-van Ekenstein rearrangement. Structure, occurrence and importance of deoxysugars, aminosugars and dihydrosugars. Sequencing of different sugar units; linkages between two or more sugar units with special reference to occurrence, structure and conformations of sucrose, lactose, maltose, raffinose, starch, cellulose and glycogen. Reducing and non-reducing sugars. Detection of sugars by chemical and chromatographic methods.

### **TERPENES AND TERPENOIDS**

General introduction and classification, Isoprene rule, general methods of determining the structure. Monoterpenes: acyclic; chemistry and synthesis of myrcene, citral and geraniol, monocyclic;  $\alpha$ -terpenol, bicyclic; chemistry and synthesis of  $\alpha$ -pinene and camphor. Diterpenes; gibberellins chemistry and structural determination using spectroscopic methods.

### **STEROIDS**

Introduction to steroids. Cholesterol; Occurrence, isolation, physical properties, medicinal importance. Structural elucidation by chemical methods; structure and molecular formula, reactions with acetic anhydride, reduction with  $H_2/Ni$ , oxidation with  $CrO_3$  and  $Se$ , size of the rings (Blanc's rule), position of hydroxyl group and double bond, hydroxyl group and double bond in different rings, nature and position of side chain, position of angular methyl groups, stereochemistry of cholesterol. Structural elucidation by spectroscopic methods; IR, UV, Mass,  $^1H$ -NMR and  $^{13}C$ -NMR spectroscopy.

### **PRACTICALS**

Synthesis of m-dinitrobenzene from nitrobenzene.

Synthesis of m-nitroaniline from aniline.

Synthesis of acetanilide from aniline.

Synthesis of p-nitroacetanilide from acetanilide.

Synthesis of p-nitroaniline from p-nitroacetanilide.

Synthesis of benzoin from benzaldehyde.

Synthesis of benzil from benzoin.

Synthesis of benzilic acid from benzyl.

Synthesis of dibenzalacetone from benzaldehyde and acetone.

### **BOOKS RECOMMENDED**

1. Finar IL "Organic Chemistry" Vol I and II 5<sup>th</sup> Ed (1988) Longman England
2. Shoppe CW "Chemistry of Steroids" 2<sup>nd</sup> Ed (1964)
3. Percival EGV, Garnet J "Structural Carbohydrate Chemistry" (1985) Miller Ltd, London
4. Collins PM "Carbohydrates" (1987) Chapman and Hall, London
5. Cordell GA "Introduction to Alkaloids" (1981) John Wiley and sons. Inc
6. Manske RHF "The Alkaloids Chemistry and Physiology" Vol VIII (1960) Academic Press, Inc
7. Manske RHF "The Alkaloids Chemistry and Physiology" Vol XVI (1977) Academic Press, Inc
8. Mann FG, Saunders BC "Practical Organic Chemistry" (1975) Lowe and Brydone (printers) Ltd, Thetford, Norfolk
9. Vogel AI "Text Book of Practical Organic Chemistry" 5<sup>th</sup> Ed (1994) Longman Group Ltd

### **CHM-552 PHYSICAL CHEMISTRY**

Credit hours: (2+1)

#### **CLASSICAL THERMODYNAMICS**

Definitions and Classification of Thermodynamics. Laws of Thermodynamics and relationship between thermodynamics and transport. Heat capacity and relation between  $C_p$  and  $C_v$ . Approach to reversible transformation, Thermodynamic definition of entropy, computing entropy and Free energy change. Stability criteria, Energy function and Maxwell's relationship. Derivation of thermodynamic identities. Equation of state. Phase diagram and stability of a single component system. Phase transition and critical phenomena. Thermodynamics of multi-component mixtures. Phase equilibria and the Phase rule. Fugacity ( $f$  and  $f_1$ ) and fugacity coefficient ( $\phi$  and  $\phi_1$ ). Activity and activity coefficients.

#### **CHEMICAL KINETICS**

Third and higher order reactions. Deduction of third order reactions with same and different initial concentrations of the reactants. Rate expression of  $2A+B \longrightarrow$  Products. Relation between rate equations for the forward and backward reactions. Reversible first order reactions. Consecutive first order reaction. Effect of temperature on rate constant and equilibrium constant, frequency factor. Concept of steric and energy factor. Arrhenius parameters for biomolecular reactions. Metathesis reactions not involving atoms. Association reactions of radicals. Hinshelwood theory of unimolecular reaction. Bimolecular

collision theory. Trimolecular reactions. Branched and unbranched chain reactions.

### **PHOTOCHEMISTRY**

Principles of photochemistry. Laws of photochemistry. Einstein's law of photochemical equivalence. Rates of intramolecular processes. Chemical reactions and their quantum yields. Hydrogen – bromine reaction. Hydrogen – chlorine reaction.

### **PRACTICALS**

Determination of rate constant of hydrolysis of ester in basic medium using conductometric technique.

Kinetic study of the redox reaction between iodide (I) and peroxydisulphate ( $S_2O_8^{2-}$ ) ions by initial rate, half life and isolation method. Study of the effect of solvent on kinetics of iodination of alkene by graphical method. Determination of equilibrium constant in esterification reactions. Photometric determination of the rate expression for  $MnO_4^-$  mediated organic oxidation. Kinetic study of inversion of sucrose by polarimetry.

### **BOOKS RECOMMENDED**

1. Alberty RA "Physical Chemistry" 7<sup>th</sup> Ed (1987) John Wiley and Sons, New York
2. Atkins PW "Physical Chemistry" (2002) Oxford University Press
3. Maron SH and Jeroma B "Fundamentals of Physical Chemistry" (1998) Macruthan Publishing Co. Inc, New York
4. Jones M "Elements of Physical Chemistry" (2001) Adison Sesky Publishing Co
5. Adamson AW "Understanding Physical Chemistry" 3<sup>rd</sup> Ed (2001) Benjamin Cummings Publishing Comp. Inc
6. Heald C and Smith ACK "Applied Physical Chemistry" (2003) English Language Book Society and Macmillan
7. Danniell and Alberty "Experimental Physical Chemistry" (2002) Mc Graw Hill
8. Klotz IM and Rosenberg RM "Chemical Thermodynamics Basic theory and Methods" 5<sup>th</sup> Ed (1994) John Wiley and Sons. Inc
9. Albertry RA and Silbvy RJ "Physical Chemistry" 1<sup>st</sup> Ed (1992) John Wiley and Sons. Inc
10. Woolbury G "Physical Chemistry" (1997) Brooks/Cole Publishing Company

**BS CHEMISTRY FOURTH YEAR  
ANALYTICAL CHEMISTRY  
SEMESTER-VII**

**CHM-611: STATISTICS FOR CHEMISTS AND  
INTRODUCTION TO ENVIRONMENTAL ANALYTICAL  
CHEMISTRY**

Credit Hours: (2+1)

**(A) Statistics for Analytical Chemistry**

Treatment of analytical data, application of statistics in analytical chemistry and statistical terminology; significant figures and the rules for addition, subtraction and multiplication, rounding off data, errors in quantitative analysis, types of error; accuracy and precision. Mean and the standard deviation, variance, distribution of errors, standard error of the mean, confidence limits and their use, propagation of random errors in addition, multiplication, division and other mathematical functions, propagation of systematic errors. Significance Tests: The null hypothesis, pooled and paired t-tests, one tailed and two tailed tests, F-test, detection of gross errors by various statistical tests, the chi-squared test, analysis of variance (ANOVA) one way and two way. Linear regression analysis: correlation coefficient, slope and the intercept and the calculation of standard deviation in the slope and the intercept. Quality control, control charts, the importance of range, cusum and the cusum chart. Concepts and definitions of quality control, quality assurance, good laboratory practice (GLP), quality audit and quality system review. Introduction to sampling: Design of a sampling procedure, methods of taking samples (solids, liquids and gases), statistics in sampling, monitoring the performance of analytical procedures.

**(B) Introduction to environmental chemistry**

**Introduction:** History and significance of environmental degradation, Energy resources and their environmental consequences, fossil fuels, nuclear energy, synthetic chemical fuel, emission from thermal units, nuclear waste and its disposal.

**Atmospheric Pollution:** Importance of air, nature and composition of atmosphere, temperature and pressure profiles of different layers of the atmosphere, common air pollutants and their sources, oxides of C,N, and S hydrologic cycle, green house effect.

**Water Pollution and Water Treatment:** Importance of water, physical and chemical properties of water, criteria for water quality,

BOD and COD, sources of water pollution (industrial, agricultural, municipal and natural), Fertilizers, pesticides, detergents, heavy metals and persistent organic pollutants.

**Monitoring of Environmental Pollution:** Principles, applications of analytical techniques for monitoring of pollution with special reference to GC, HPLC, UV and IR spectrometry, Atomic absorption spectroscopy. Legislation aspects of environmental pollution.

#### **BOOKS RECOMMENDED**

1. Skoog DA and Leary JJ "Principles of Instrumental Analysis" 4<sup>th</sup> Ed (1992) Saunders College Publishing
2. Spiro TG and Stigliani WM "Chemistry of the Environment" 2<sup>nd</sup> Ed (2002) Prentice Hall
3. Moore JW and Moore EM "Environmental Chemistry" Academic Press, New York
4. Manahan SE "Environmental Chemistry" 6<sup>th</sup> Ed (1994) Lewis Publishers
5. Harvey DT "Modern Analytical Chemistry" 1<sup>st</sup> Ed (2000) Mc Graw Hill New York
6. Miller JC and Miller JN "Statistics for Analytical Chemistry"
7. Ellis Harwood Series in Analytical Chemistry, 3<sup>rd</sup> Ed
8. Woodget BW, Cooper D "Samples and Standards" ACOL series

#### **CHM-621: SOLUTION CHEMISTRY AND THERMODYNAMICS**

Credit Hours: (3+0)

##### **(A) Solution Chemistry**

**Introduction:** Order chaos and equilibrium in solutions, factors affecting equilibrium, water solution of ions, the difference between equilibrium quotient and equilibrium constant, the concept of solubility as a compromise between the tendency of order and disorder and the role of energy in salvation.

**Proton Transfer Equilibrium:** Proton in aqueous solution, autoprotolysis of water and the factors affecting it, proton balance equations, relationship between pH and pQ<sub>a</sub>, graphic and algebraic treatment of aqueous equilibrium.

**Coordination Equilibrium:** reactions and definitions, factors affecting stability constant, distribution of species and distribution graphs.

**Solubility Equilibrium:** Introduction, solubility of salts with basic anions, solubility with simultaneous equilibria involving metal ions and study of complexation of cations with anions.

**(B) Thermodynamics**

**Introduction:** Molecular basis of entropy and statistical basis of the second law, the quantum of entropy changes, and the third law of thermodynamics.

**Behaviors of Heat Capacity:** Experimental and theoretical discrepancies in the heat capacity data, the need for plausible explanation and the quantum mechanical explanation of the heat capacity.

**Quantum States:** Energy levels, energy compartmentalized into translation, rotation, and vibrational energies, equations for computing these energies, the concept of microstates and derivation of Boltzmann distribution law.

Determination of the Partition Functions: Localized and non-localized systems, partition function specific to energy segments, Sackur-Tetrode equation, equation for calculating vibrational and translational partition functions, relation between partition functions and equilibrium constant.

**BOOKS RECOMMENDED**

1. Thomas and Blackburn R "Equilibrium: A Chemistry of Solutions" (1969) Holt Rinehart and Winston Inc
2. DeFord DD "The Reliability of Calculations based Upon the Law of Chemical Equilibrium" J Chem Education (1954) 31, 460
3. Gasser RPH and Richards WG "Entropy and Energy Levels" (1974) Oxford University Press
4. Wyatt PAH "The Molecular Basis of Entropy and Chemical Equilibrium" (1971) Royal Institute of Chemistry, London
5. Seddon JM and Gale JD "Thermodynamics and Statistical Mechanics" (2002) Royal Society of Chemistry, UK

**CHM-631: SPECTROSCOPY -I**

Credit Hours: (3+0)

**Nuclear Magnetic Resonance Spectroscopy**

Background & principles: Introduction to nuclear magnetic resonance; chemical shifts; spin-spin splitting (spin coupling); relaxation times

Instrumentation: Magnets; sample probes; Radiofrequency sources detectors; techniques in instrumentation, sample handling; NMR solvents; purity; reference compounds (TMS etc), Quantitative aspects:  $^1\text{H}$  NMR: Interpretation; structural elucidation; concept of isotopomers isotopic substitution.  $^{13}\text{C}$  NMR: Interpretation; structural elucidation; concept of isotopomers isotopic substitution Multi-nuclear NMR:  $^{19}\text{F}$ ,  $^{31}\text{P}$ ,  $^2\text{H}$ ,  $^{11}\text{B}$ ,  $^{129}\text{Xe}$ ,  $^{79}\text{Br}$ ,  $^{81}\text{Br}$  NMR and other NMR active nuclei

### **Electron Spin Resonance Spectroscopy**

Background and principles of ESR, Comparison with NMR; Instrumentation; Nuclear hyperfine splitting; Quantitative aspects; Energy level diagram; presentation of spectra, Spin trapping technique; isotopic substitution, application of ESR in structure elucidation, Spectra of organic free radicals and spectra of radical containing hetero-atoms

### **Spectra of Transition Metal Complexes**

Quantum numbers and shapes of orbital (spin angular momentum, angular momentum, resultant angular momentum, inter-electronic repulsion and its parameters, (Russell-Saunders coupling) Spin states, Terms, Spin multiplicity. Electronic transitions in metals Spectra of octahedral and tetrahedral symmetries, Charge transfer spectra. Analysis of spectra for different  $d^n$  configurations in octahedral and tetrahedral ligand fields and fields of lower symmetry. Hole formalism Use of Orgel, Tanabe-Sugano and energy-ratio diagrams. Analysis of band shapes and intensities, Jahn-Teller effects, spectral assignments and derivation of ligand field parameters. Spectrochemical and nephelauxetic series

### **BOOKS RECOMMENDED**

1. Macomber RS "NMR Spectroscopy: Basic Principles and Applications" 1<sup>st</sup> Ed (1988) Harcourt
2. Bunce and Nigel "Introduction to the Interpretation of Electron Spin Resonance Spectra of Organic Radicals" (1987 ) Journal of Chemical Education 64, 907
3. Drago RS "Physical Methods in Inorganic Chemistry" (1965) Van Nostrand Reinhold
4. Sutton D "Electronic Spectra of Transition Metal Complexes" (1968) Mc Graw Hill.
5. Skoog AD, Holler FJJ and Nieman TA "Principles of Instrumental Analysis" 5<sup>th</sup> Ed (1997) Saunders College Publishing, New York

6. Willard HH, Merritt LL, Dean JA and Settle FA "Instrumental Methods of Analysis" 7<sup>th</sup> Ed (1988) Wadsworth Publishers
7. Christian GD and O'Reilly JE "Instrumental Analysis" 2<sup>nd</sup> Ed (1986) Allyn and Bacon, Inc

### **CHM-641: INSTRUMENTAL METHODS OF ANALYSIS**

Credit Hours: (0+ 3) (**Laboratory Course**)

This laboratory course would be based on the introduction of fundamental techniques of instrumental analysis. The instruments include single beam spectrophotometer, double beam spectrophotometer, atomic absorption spectrophotometer, fluorimeter, ion chromatograph and high performance liquid chromatograph and introduction to statistical treatment of analytical data.

Determination of wavelength of maximum absorption, construction of calibration curves by Beer's law, standard addition method, Internal standard method, photometric titrations, simultaneous determination of metals ions, Determination of metal-to ligand ratio by Job's plot and molar ratio method, trace analysis by atomic absorption using flame, hydride generation for As and cold vapor technique (for Hg), fluorometric determination of acetylsalicylic acid in analgesic tablets, analysis of mixture by HPLC or ion chromatography.

### **BOOKS RECOMMENDED**

1. Christian GD "Analytical Chemistry" 6<sup>th</sup> Ed (2003) Wiley
2. Sawyer DT, Heineman WR and Beeb JM "Chemistry Experiments for Instrumental Methods" (1984) John Wiley and Sons
3. Harris D "Quantitative Chemical Analysis" 5<sup>th</sup> Ed (1998) W.H. Freeman and Company
4. Mendham J, Denney RC, Barnes JD and Thomas M.JK "Vogel's Quantitative Analysis" 6<sup>th</sup> Ed (2000) Prentice Hall

### **CHM-651: POTENTIOMETRY AND AMPEROMETRY**

Credit Hours: (0 + 3) (**Laboratory Course**)

#### **Potentiometry: Neutralization Reactions**

- Titration of acid mixtures
- Determination of mineral acid in a given vinegar solution
- Determination of ascorbic acid in a vitamin tablet
- Determination of acetylsalicylic acid in analgesic tablets
- Determination of folic acid in a given tablet

- Determination of dissociation constant of different weak acids using Henderson-Hasselbalch equation.
- Determination of dissociation constants of polybasic acids
- Simultaneous determination of chromate and dichromate in a mixture
- Determination of solubility product, Gibbs free energy and enthalpy for the dissolution of calcium hydroxide.
- Study of complexation reactions of copper, nickel and cobalt with EDTA
- Determination of percentage purity of sodium carbonate in commercial soda ash.

#### **Potentiometry based on redox titrations of different systems**

- Standardization of potassium permanganate with KI
- Precipitation and complexation reactions
- Determination of Fe(III) with EDTA
- Determination of formal potential,  $K_{(equilb)}$  and “n” of some redox systems

#### **Amperometry**

- Verification of Randles Sevcik equation for different redox systems
- Construction of calibration curve between diffusion current and concentration of analyte.
- Amperometric titration of some redox systems

#### **BOOKS RECOMMENDED**

1. Braun RD "Introduction to Instrumental Analysis" (1987) Mc Graw Hill, New York
2. Mendham J, Denney RC, Barnes JD and Thomas MJK "Vogel's Quantitative Analysis, Prentice Hall, 6<sup>th</sup> Ed (2000)
3. Sawyer DT, Heineman WR and Beeb JM "Chemistry Experiments for Instrumental Methods" (1984) John Wiley & Sons
4. Harris D "Quantitative Chemical Analysis" 5<sup>th</sup> Ed (1998) W. H. Freeman and Company
5. William EB, Louis KJ and Ben R "Determination of  $K_{sp}$ ,  $\Delta G$ ,  $\Delta H$ , and  $\Delta S$  for the Dissolution of Calcium Hydroxide in Water: A General Chemistry Experiment" (2000) J Chem Education 77, 1039
6. Kalbus LH, Petrucci RH, Forman JE and Kalbus GE "Titration of Chromate- Dichromate Mixtures" (1991) J Chem Education 68, 677

## SEMESTER-VIII

### **CHM-612: ELECTRONICS AND MASS SPECTROMETRY**

Credit Hours: (3+0)

#### **(A) Electronics**

**Introduction:** conductors, insulators, charge, electric field, potential, potential difference, current, electron flow, conventional current, direct and alternating current, hole charge, resistance and resistors, open and closed circuits.

Resistors and resistance: Color coding, factors affecting resistance, Ohms law, concept of power and units.

**Circuit Symbols and circuits:** Symbols of components of circuits, series circuits and parallel circuits, combination of series and parallel circuits, Kirchoff Voltage law, Kirchoff Current law, Wheat stone bridge, fuse and its types. Methods of solving circuits: Mesh circuit analysis, method of branch current, Node voltage analysis.

**Capacitors:** Series and parallel capacitors and circuit capacitor reactance. Ohms law as applied to capacitance current.

**Electricity and magnetism:** Definition and units of magnetic flux, flux density, Induction, permeability, relay, Classification of magnetic material. Magnetomotive force, ampere turns, field intensity, Ohms law for magnetic currents. Magnetic field around a conductor, right hand rule, magnetic polarity, motor action, induced current, Faraday's law.

**Generation of AC current:** Methods and principles, AC wave forms, Induction by AC currents, mutual inductance, Transformers, Inductive reactance, RC and L/R time constant AC circuits. Filters, High pass Low pass filters, RC band pass, Band stop filters.

**Semiconductors:** p-n junctions, Applications, working of transistors and their uses.

**Binary Digits, Logic gates and Boolean Algebra:** Binary to decimal and vice versa, Hexadecimal system, Hexadecimal to binary, binary coded decimal, binary arithmetic (addition subtraction and multiplication).

Logic gates: NOT gate, OR gate, AND gate, NOR, NAND, XOR, XNOR (symbols, construction of truth table). Boolean algebra: Combination of the above circuits, read out devices, LEDs, LCDs, Modulation of AM and FM.

**Operational amplifier:** Feed back, Voltage etc.

**Signal conversion:** Analogue signals, Digital signals, analogue to digital, digital to analogue conversion, In-line, On-line and Off-line systems, Components of personal computers, software classification, integrator, controller. Signal to noise ratio: Definition and scope

### **(B) Mass Spectrometry**

Definitions: mass, mass-to-charge ratio, resolution, accuracy, isotope distributions. Theoretical principles, Ionization processes: EI, CI, FAB, MALDI. Instrument components: Mass analyzers: sectors, time-of-flight, quadrupole, ion traps MS/MS and tandem instruments. Behaviour of various classes of compounds in mass spectrometry and interpretation of mass spectra and applications to chemical analysis.

### **BOOKS RECOMMENDED**

1. Grob B "Basic Electronics" 8<sup>th</sup> Ed (1997) McGraw Hill
2. Petruzella FD "Essentials of Electronics" 2<sup>nd</sup> Ed (1999) Mc Graw Hill
3. Skoog AD, Leary JJ "Principles of Instrumental Analysis" 4<sup>th</sup> Ed (1992) Saunders College Publishing
4. Barker J and Ando DJ "Mass Spectrometry" Analytical Chemistry by Open Learning 2<sup>nd</sup> Ed (1998)
5. Hoffmann E and Stroobant V "Mass Spectrometry: Principles and Applications" Wiley 2<sup>nd</sup> Ed (2001)
6. Silverstein RM, Webster FX and Kiemle D "Spectrometric Identification of Organic Compounds" 7<sup>th</sup> Ed (2005) John Wiley and Sons.

### **CHM-622: ELECTROANALYTICAL CHEMISTRY AND INTRODUCTION TO ANALYTICAL SEPARATION**

Credit Hours: (3 + 0)

#### **(A) Electroanalytical Chemistry**

**Electrical Double Layer:** Interface, interphase, a look into the interphase, OHP and IHP, contact adsorption, Gibbs surface excess, potential differences across metal solution interfaces, outer and surface potentials difference, electrochemical potential difference, interfacial tension, electrocapillary thermodynamics, Lippmann's equation, Helmholtz- Perrin model, Guoy- Chappmann model, Stern model and Bockris-Devanathan-Muller model, charge density, differential capacitance, shape of charge capacitance curve, and the capacitance hump.

**Electrode Kinetics:** Electrochemical devices, charge transfer process in the presence and absence of electrical field, the overpotential, Butler-Volmer Equation, the idea of equilibrium exchange current density, the symmetry factor, high field and low field approximations, Tafel equation and Nernst equation. Introduction to electroanalytical techniques, review of electrochemical cells, cell potentials, electrode potentials, currents in electrochemical cell, types of electroanalytical methods.

**Non-Potentiometric Electroanalysis**

Polarography and voltammetry, electrodes, polarographic principles, excitation signals in voltammetry, linear scan voltammetry, pulse polarographic and voltammetric methods, stripping methods, and cyclic voltammetry.

**(B) Introduction to Analytical Separations**

Introduction to various separation techniques (precipitation, distillation, extraction, lyophilization and chromatography)

**High Performance Liquid Chromatography**

Instrument, stationary phases, mobile phases, HPLC columns, applications of HPLC

**Gas Chromatography**

Instrument, stationary phases, mobile phases, GC columns, types of detectors, application of GC.

**BOOKS RECOMMENDED**

6. Bockris JOM and Reddy AKN "Modern Electrochemistry" Vol I and II , 4<sup>th</sup> Ed. (2003) Plenum Press, London.
7. Bockris JOM and Drazic D "Electrochemical Science" (1972) Taylor and Francis, London
8. Bockris JOM, Bonciocat N and Guttmann F "An introduction to Electrochemical Science" (1974) Wykeham Publication, London
9. Bockris JOM and Fredlein RA "A Workbook of Electrochemistry" (1973) Plenum Press, New York
10. Skoog AD, Holler FJJ and Nieman TA "Principles of Instrumental Analysis" 5<sup>th</sup> Ed (1997) Saunders College Publishing, New York  
Snyder LR and Kirkland JJ "Introduction to Modern Liquid Chromatography" 2<sup>nd</sup> Ed (1979) Wiley-Interscience

## **CHM-622.1: PHARMACEUTICAL CHEMISTRY (OPTIONAL, IN LIEU OF 622)**

Credit Hours: (3+0)

### **Transformation of Chemicals into Drugs**

Physiochemical Properties In Relation To Biological Action: Complex events between drug administration and drug action. Solubility, partition coefficient and drug-receptor interactions

Factors Influencing Dosage Formations: Disintegration, dissolution and absorption of drugs, their pre-requisites, Effective blood level, Placebo effects, MIC values etc. and Drug-drug interactions

Drug Metabolism: Factors influencing metabolism of drugs. Site of metabolism, Metabolic changes in GI tract, Types of metabolic reactions and Reactions based on functional groups.

Structure-Activity Relationship (SAR): Chemical structure in relation to biological activity of molecules, stereochemical factors, prodrugs, isosters and pharmacophore groups.

### **Synthesis, physical and chemical properties, mode of action, SAR studies and toxicity of the following drugs**

Sulfa drugs: Sulfa drugs in current therapy (human and veterinary use).

Drugs acting on NIDDM: Sulfonylureas. Antibiotics: Penicillin and related compounds, cephalosporins, tetracyclines chloramphenicol and quinolones. Antiviral agents and antineoplastic agents. Histamines and antihistamines: H<sub>1</sub> and H<sub>2</sub>-receptor antagonists, development of H<sub>3</sub> receptors and proton pump inhibitors.

Anti-malarial drugs, Analgesics (peripheral as well as centrally acting), local anesthetics

**Recent trends in drug development:** Quantitative structure activity relationship (QSAR), computer models and stimulations with examples including a case study of at least one drug.

### **BOOKS RECOMMENDED**

1. Burger A "Medicinal Chemistry" 4<sup>th</sup> Ed Wiley Interscience New York
2. Burger A "Medicinal Chemistry" 5<sup>th</sup> Ed Wiley Interscience New York
3. Gisvold W and Lippincott Doerge "A Text Book of Organic Medicinal and Pharmaceutical Chemistry" 9<sup>th</sup> Edition

4. Korolkovas and Burckhaliter "Essentials of Medicinal Chemistry"  
Wiley Interscience New York
5. Jenkins GL et al. "The Chemistry of Organic Medicinal Products"  
Wiley Interscience New York
6. Clarks ECG "Isolation and Identification of Drugs" Vol I and II  
The Pharmaceutical Press, London

### **CHM-632: SPECTROSCOPY –II**

Credit Hours: (3+0)

#### **UV-Visible Spectroscopy**

Energy transitions in molecules, types of electronic transitions in molecules ( $n-\pi^*$ ,  $\pi-\pi^*$ ,  $\sigma-\sigma^*$  etc.), selection rules, Beer's Lambert law and electronic spectra, explanation of bathochromic, hypsochromic shifts, fundamentals of the optical components of spectrometers, radiation sources, monochromators based on Czerny Turner mounting, and echelle gratings, detectors, photometric accuracy and high precision techniques, spectrophotometric errors, analysis of multicomponent analysis and derivative spectroscopy, diode array spectrophotometers.

#### **Infrared Spectrophotometry**

Interaction of infrared radiation with molecules, types of molecular vibrations, selection rules, instrumentation, optical materials, sources, detectors used in IR spectroscopy. Interferometric (Fourier Transform) spectrophotometers, calibration and standardization and preparation of samples for the analysis of solids, liquids and gases

#### **Luminescence Spectrometry (Fluorescence, Phosphorescence & Chemiluminescence):**

Introduction, types of luminescence, energy levels in luminescent molecules, Process involving excited states i.e. absorption, vibrational relaxation, internal conversion, fluorescence, intersystem crossing and phosphorescence. Instrumentation for fluorescence measurements and phosphorescence measurements, excitation and emission spectra, luminescence efficiency and factors affecting it, post and pre-filter effects. Mathematical relationship between luminescence and concentration and analytical applications

#### **Atomic Spectroscopy**

##### **(a) Atomic Absorption: Flame and Electrothermal Atomization Methods**

Sample atomization, types and sources of atomic spectra, radiation sources (Hollow cathode lamp, Electrode discharge lamp), burners and

nebulizers, atomization cells (flames and graphite furnace), atomic absorption spectroscopy, flame emission spectroscopy. Interferences and their control, cold vapor for mercury and hydride generation techniques for trace analysis of metals. Background correction by deuterium lamp, Smith Hieftje technique and Zeeman effect.

**(b) Emission spectroscopy**

Use of Grotrian diagram, the phenomenon of flame emission and interferences encountered in flame emission, emission spectroscopy based on plasma sources and ICP spectrometer, simultaneous analysis of elements by ICP

**BOOKS RECOMMENDED**

1. Skoog AD, Holler FJJ, Nieman TA "Principles of Instrumental Analysis" 5<sup>th</sup> Ed (1997) Saunders College Publishing, New York
2. Willard HH, Merrit LL, Dean JA and Settle FA "Instrumental Methods of Analysis" 7<sup>th</sup> Ed (1988) Wadsworth Publishers
3. Christian GD, O'Reilly JE "Instrumental Analysis" 2<sup>nd</sup> Ed (1986) Allyn and Bacon, Inc
4. Rousseac F and Rousseac A "Chemical Analysis-Modern Instrumentation Methods and Techniques" (2000) Wiley
5. Braun RD "Introduction to Instrumental Analysis" (1987) Mc Graw Hill, New York
6. Strobel HA "Chemical Instrumentation: Systematic Approach to Instrumental Analysis" (1989) Wiley, New York
7. Banwell CN and Mc Cash EM "Fundamentals of Molecular Spectroscopy" (1994) Tata Mc Graw Hill

**CHM-642: CLASSICAL METHODS OF CHEMICAL ANALYSIS**  
Credit Hours (0+3) (**Laboratory Course**)

This laboratory course is based on the analysis of real samples using mainly titrimetric and gravimetric methods of analysis. The techniques include neutralization titrations, redox titrations, complexometry, ion-exchange chromatography and gravimetry.

- Determination of acetic acid in vinegar.
- Calcium in eggshell by back titration.
- Determination of magnesium hydroxide in milk of magnesia.
- Calcium in milk by EDTA back-titration
- Analysis of copper by complexometric titration.
- Analysis of a mixture of Mg and Mn by EDTA
- Temporary and Permanent hardness of water.

- Determination of copper by iodometry.
- Determination of ascorbic acid in vitamin tablets
- Determination of sodium hypochlorite in commercial bleach by iodometry
- Winkler titration for the determination of oxygen in water
- Separation of two cations by anion exchange chromatography.
- Total cations in water by cation exchange chromatography.
- Gravimetric determination of copper as CuO.
- Homogenous precipitation of Fe as Fe<sub>2</sub>O<sub>3</sub>.

Other new experiments will be incorporated depending upon the availability of reagents and apparatus.

**Weekly Seminars and Student Presentations:** Based on theoretical and practical topics related to titrimetry, gravimetry, laboratory safety and proper usage and calibration of laboratory glassware.

#### **BOOKS RECOMMENDED**

1. Laitinen, HA "Chemical Analysis: An Advanced Text and Reference" (1960) Mc Graw Hill, New York
2. Harris D "Quantitative Chemical Analysis" 5<sup>th</sup> Ed (1998) W.H. Freeman and Company
3. Mendham J, Denney RC, Barnes JD and Thomas MJK "Vogel's Quantitative Analysis" 6<sup>th</sup> Ed (2000) Prentice Hall
4. Mendham J, Dodd D and Cooper D "Classical Methods" Vol I and II (1987) (ACOL series) London

#### **CHM-652 CLINICAL METHODS OF ANALYSIS AND ENVIRONMENTAL ANALYTICAL CHEMISTRY**

Credit Hours: (0 + 3) (**Laboratory Course**)

- Quantitative analysis of Na<sup>+</sup>, K<sup>+</sup>, Ca<sup>2+</sup>, Cl<sup>-</sup> and inorganic phosphorus in serum.
- Analysis of serum glucose by o-toluidine and copper reduction method.
- Analysis of NPN i.e. creatinine, urea-N and uric acid in serum.
- Determination of serum cholesterol concentration.
- Analysis of serum iron and TIBC.
- Determination of protein (total, albumin and globulin) in serum.
- Analysis of salicylate in serum.
- Determination of serum amylase activity.
- Determination of hemoglobin (as oxyhemoglobin and cyanomethemoglobin).

- Analysis of mercury in urine.
- Determination of concentration of lead in blood.

**Environmental Analytical Chemistry experiments based on:**

Soil, sludge, sediment and dust, analysis, analysis of plant materials, determination of organic pollutants in water by gas/liquid chromatography, analysis of toxic heavy metals in environmental samples by atomic absorption or emission spectroscopy.

**BOOKS RECOMMENDED**

1. Nobert and Tietz W "Textbook of Clinical Chemistry" 2nd Ed (1994) WB Saunders Company, Philadelphia
2. Kaplan A and Szabo LL "Clinical Chemistry: Interpretation and Techniques" 3<sup>rd</sup> Ed (1988) Lea and Febiger, Philadelphia
3. Bender GT "Principles of Chemical Instrumentation" (1987) WB Saunders Company, Philadelphia



## **INORGANIC CHEMISTRY**

### **SEMESTER- VII**

#### **CHM-617: KINETICS AND MECHANISM OF INORGANIC REACTIONS**

**Credit Hours: (3+0)**

Revision of Basic Concepts of Reaction Kinetics with Particular Reference to the Effect of Concentrations of Reacting Species (Order of Reaction) Temperature and Pressure (Entropy, Enthalpy and Volume of Activation), Ionic Strength and Diffusion Controlled Rates. Methods of Measurement of Reaction Rates of Slow Reactions, Initial Rate Methods, Absorbance, Conductance and other Conventional Techniques. Fast Reactions Using Stopped-flow, Pulse Radiolysis, Flash Photolysis and Relaxation Methods (T-jump and p- jump). Rate Law and Reaction Mechanism, Single and Multi Term Rate Laws, Fractional and Inverse Order Reactions and their Implications on Mechanism. Steady- State Approximation and Rapid Equilibrium Prior to Rate Determining Step.

Dissociative and Interchange Mechanisms. Effects of Non-Labile Ligands, Field Considerations, Solvent Effects, Activation Parameters. Selected Examples from Octahedral and Square Planar Systems. Oxidation Reduction Reactions Precursor & Successor Complexes Inner-Sphere & Outer-Sphere Electron Transfer Reactions. Factors Contributing to Activation Energy in the Pre-Exponential and Exponential Terms. Adiabatic and Non-Adiabatic Electron Transfer, Marcus-Hush Theory.

Catalysis (Homogeneous and Heterogeneous) of Organic Reactions by Inorganic Systems. 16 and 18 Electron Rule, Oxidative Addition, Reductive Elimination and Free Radical Mechanisms. Selected Examples.

Photochemistry; Key Definitions (Fluorescence, Phosphorescence) Inter System Crossing, Quantum Efficiency, Einstein, Stern-Volmer Plots etc.) Jablonski's Diagram Modes of Excitation of Transition Metal Complexes.

Selection Rules: Thermal and Anti-Thermal Substitution Reactions, Photo Chemically Induced Redox Reactions. Attempts to Split Water Molecule for H<sub>2</sub> Production Using Solar Energy.

#### **BOOKS RECOMMENDED**

1. Shriver DF, Atkins PW and Langford CH "Inorganic Chemistry" (1994) Oxford University Press
2. Cotton FA, Wilkinson G, Murillo CA and Bochmann M "Basic Inorganic Chemistry" 2<sup>nd</sup> Ed (1987) John Wiley and Sons, Inc
3. Holliday K and Massey AG "Inorganic Chemistry in Non-Aqueous Solvents" (1985) Pergamon Press
4. Bond GC "Heterogeneous Catalysis" 2<sup>nd</sup> Ed (1987) Clarendon Press Oxford
5. John B "Metal Ions in Solution" (1978) Chichester Ellis Howard
6. Cox and Camp TJ "Introduction of Photochemistry" (1971) McGraw Hill New York
7. Richard PW "Principles and Applications of Photochemistry" (1988) Oxford University Press
8. Atwood JD "Inorganic and Organometallic Reaction Mechanisms" 2<sup>nd</sup> Ed (1950) Wiley VCH

- Jordan RB "Reaction Mechanism of Inorganic and Organometallic Systems" 2<sup>nd</sup> Ed (1991) Oxford University Press, Inc

### **CHM-627: CHARACTERIZATION OF METAL COMPLEXES**

Credit Hours: (3+0)

#### ***(i) Symmetry and Group Theory***

Symmetry Elements and Symmetry Operations, Point Groups and Classification of Molecules According to Point Group, Multiplicity Rule, Character Table and its Importance, Reducible and Irreducible Characters, Applications of Group Theory on Atomic Orbitals and Molecular Orbitals, Detection of Hybrid Orbitals by Group Theory, Reducible Representations and Prediction of I. R. and Raman Spectra and their Selection Rules, Prediction of Chirality and Optical Activity of the Molecules by Using their Point Groups.

#### ***(ii) Magnetic Properties of the Metal Complexes***

The Importance of Magnetism in Transition Element Chemistry, Origin of Paramagnetic Moment, Diamagnetism, Magnetic Susceptibility, Magnetic Moments from Magnetic Susceptibility, Ferromagnetism and antiferromagnetism in complexes.

#### **BOOKS RECOMMENDED**

- Shriver DF, Atkins PW and Langford CH "Inorganic Chemistry" (1994) Oxford University Press
- Hill JW and Petrucci RH "General Chemistry" (1996) Prentice-Hall Inc
- Cotton FA, Wilkinson G, Murillo CA and Bochmann M "Advanced Inorganic Chemistry" (1999) John Wiley and Sons, Inc
- Basolo F and Johnson RC "Coordination compounds: The Chemistry of Metal Complexes" (1964) W. A. Benjamin, Inc
- Kettle SFA "Coordination compounds" (1969) Thomas Nelson and Sons, Ltd

Credit Hours: (3+0)

(i) Material Science

The International Tables for Crystallography, Close Packing and Eutactic Structures Framework Nets and Topologies of Extended Solids, Powder Diffraction I - Peak Positions, Powder Diffraction II - Peak Intensities, Electrostatic Interactions & Ionic Bonding, Pauling's Rules and The Bond Valence Method, Atomic Orbitals, Periodic Trends and Covalent Bonding, Molecular Orbital (MO) Theory, Band Theory (LCAO Approach), Electronic Conductivity: Metals and Semiconductors, Optical Properties I: Gemstones & Pigments, Optical Properties II: Phosphors, Lasers & Displays. Magnetism & Magnetic Materials. Dielectric Properties and Materials. Ionic Conductivity & Solid Electrolytes Solid Electrolytes: Batteries, Fuel Cells and Sensors. Transition Metal Oxides I: Perovskites. Transition Metal Oxides II: Rock Salt and Rutile.

(ii) Marine Chemistry

Introduction to Oceanography; Marine Chemistry and Geochemistry; Physical and Chemical Properties of Sea Water, Organic Matter and Energy Fluxes, Carbon Dioxide Intake and Transformation, Major Minor and Trace Inorganic and Organic Constituents in Sea Water and Sediments and their Impacts on Biota; Renewable Energy Sources, Industrial and Environmental Aspects of Arabian Sea. Geochemistry and geochemical distribution of elements in coastal areas of Pakistan.

**BOOKS RECOMMENDED**

1. Weller MT "Inorganic Material Chemistry" (1994) Oxford Science Publications, Oxford University Press
2. Shriver DF, Atkins PW and Langford CH "Inorganic Chemistry" (1994) Oxford University Press
3. Olmsted J and Williams GM "Chemistry: The Molecular Science" 1994) Mosby-Year Book, Inc
4. Buchner W, Schliebs R and Winter G "Industrial Inorganic Chemistry" (1989) KH Buchel
5. Perry "Chemical Engineering Hand Book" 3<sup>rd</sup> Ed (1950) Mc Graw Hill Inc, New York
6. Hester RE, Harrison RM "Chemistry in the Marine Environment" (2000) Royal Society of Chemistry

7. Millero FJ "Chemical Oceanography" 3<sup>rd</sup> Ed (2005) CRC Press
8. Sammartano S, Gianguzza A and Pelizzetti E "Chemistry of Marine Water and Sediments" 1<sup>st</sup> Ed (2002) Springer

#### **CHM-647: INSTRUMENTAL METHODS OF ANALYSIS**

Credit Hours: (0+3)

This laboratory course would be based on the introduction of fundamental techniques of instrumental analysis. The instruments include single beam spectrophotometer, double beam spectrophotometer, atomic absorption spectrophotometer, fluorimeter, ion chromatograph and high performance liquid chromatograph and introduction to statistical treatment of analytical data. Determination of wavelength of maximum absorption, construction of calibration curves by Beer's law, standard addition method, Internal standard method, photometric titrations, simultaneous determination of metals ions, Determination of metal-to ligand ratio by Job's plot and molar ratio method, trace analysis by atomic absorption using flame, hydride generation for As and cold vapor technique (for Hg), fluorometric determination of acetylsalicylic acid in analgesic tablets, analysis of mixture by HPLC or ion chromatography.

#### **BOOKS RECOMMENDED**

1. Harris D "Quantitative Chemical Analysis" 5<sup>th</sup> Ed (1998) W. H. Freeman and Company
2. Mendham J, Denney RC, Barnes JD and Thomas MJK "Vogel's Quantitative Analysis" 6<sup>th</sup> Ed (2000) Prentice Hall
3. Marr G and Rockett BW "Practical Inorganic Chemistry" (1972) Van Nostrand Reinhold Company
4. Pass G and Sutcliffe H "Practical Inorganic Chemistry: Preparations, Reactions and Instrumental Methods" 2<sup>nd</sup> Ed (1974) Chapman and Hall
5. Pass G and Sutcliffe H "Practical Inorganic Chemistry: Preparations, Reactions and Instrumental Methods" 3<sup>rd</sup> Ed (1985) Chapman and Hall

#### **CHM-657: CLASSICAL METHODS OF ANALYSIS**

Credit Hours: (0+3)

1. Analysis of Caustic Soda, Washing Soda,  $\text{Fe}^{+2}$ ,  $\text{Fe}^{+3}$  in a Mixture,  $\text{Fe}^{+2}$ ,  $\text{Fe}^{+3}$  and  $\text{Al}^{+3}$  in a Mixture,  $\text{H}_2\text{O}_2$  as Oxidizing Agent,  $\text{H}_2\text{O}_2$  as Reducing Agent,  $\text{HCl}$  and  $\text{H}_2\text{SO}_4$  in a Mixture,  $\text{HCl}$  and  $\text{H}_3\text{BO}_3$  in a Mixture,  $\text{H}_2\text{SO}_4$  and  $\text{H}_2\text{C}_2\text{O}_4 \cdot 2\text{H}_2\text{O}$  in a Mixture,  $\text{Ca}^{+2}$  and  $\text{Mg}^{+2}$  in a Mixture,  $\text{H}_2\text{SO}_4$ ,  $\text{H}_2\text{C}_2\text{O}_4 \cdot 2\text{H}_2\text{O}$  and  $\text{Na}_2\text{C}_2\text{O}_4 \cdot 2\text{H}_2\text{O}$  in a Mixture.
2. Determination of Formula of an Unknown Compound.

#### **BOOKS RECOMMENDED**

1. Jeffery GH, Bassett J, Mendham and Denny RC "Vogel's Textbook of Quantitative Chemical Analysis" 5<sup>th</sup> Ed (1989) Longman group UK Ltd
2. Marr G and Rockett BW "Practical Inorganic Chemistry" (1972) Van Nostrand Reinhold Company
3. Pass G and Sutcliffe H "Practical Inorganic Chemistry: Preparations, Reactions and Instrumental Methods" 3<sup>rd</sup> Ed (1985) Chapman and Hall
4. Wesly WE "Industrial Water Pollution Control" (2000) Mc Graw Hill New York

#### **SEMESTER- VIII**

CHM-618: APPLICATIONS OF INSTRUMENTAL TECHNIQUES  
Credit Hours: (3+0)

Electron Spin Resonance Spectroscopy: Theory, Various Techniques, Applications and Problems related to ESR.

Nuclear Magnetic Resonance Spectroscopy: Theory, Techniques, Applications and Problems related to NMR.

Rotational and Vibrational Spectroscopy: Infra red and Raman Spectroscopy Theories and derivation of related equations. Characterization of complexes with respect to IR and Raman Spectra. Detection of Functional Groups and study of Finger Print Region.

UV-Visible Spectra of Transition Metal complexes with Reference to d-d Transitions. Interpretation of Spectra of Complexes with the help of Tanabe Sugano Diagram.

Basics of Chromatography; Applications off Thin Layer Chromatography (TLC), High performance Liquid Chromatography HPLC, and Gas Chromatography (GC) to various inorganic and organometallic compounds.

**BOOKS RECOMMENDED**

1. Lee JD "Concise Inorganic Chemistry" Chapman and Hall 5<sup>th</sup> Ed (1995)
2. Shriver DF, Atkins PW, and Langford CH "Inorganic Chemistry" (1994) Oxford University Press
3. Harrington TJ and Earnshaw A "The Chemistry of the Transition Elements" (1973) Oxford University Press
4. Banwell CN "Fundamentals of Molecular Spectroscopy" (1983) Tata McGraw Hill New Delhi
5. Pople CP "Electron Spin Resonance" (1967) John Wiley, New York
6. Choppins GR and Rayberg, J "Nuclear Chemistry and Application" 1<sup>st</sup> Ed (1989) Pergaman Press, Oxford New York
7. Barrow GM "Introduction to Molecular Spectroscopy" (1962) McGraw Hill New York
8. Ayscough PB "Electron Spin Resonance in Chemistry" (1967) Methuan and Co. London
9. Pople JA "High Resolution Nuclear Magnetic Resonance" (1959) McGraw Hill

**CHM-628: ORGANOMETALLIC COMPLEXES AND INORGANIC INDUSTRIAL CHEMISTRY**

Credit Hours: (3+0)

**(i) Organometallic Complexes**

Olefin Complexes. Cyclopentadienyl Compounds. Arene Metal Compounds Carbocyclic Compounds. Heterocyclic Sandwich Compounds. Carbene Complexes. Alkyne and Allyl Complexes and Their Spectroscopic Explanation and Characterization. Application of Molecular Orbital Theory.

**(i) Inorganic Industrial Chemistry**

Nitrogen Containing Explosive, Initiators and propellant; Zeolites and clays as sorbent; Water Conditioning, water treatment; sewage and dissolved gases treatment; Nitrogen, Phosphorus and potash in agriculture, Sulfur in Pulp and Paper Industry; Corrosion and Corrosion inhibitors; Quality and uses of salts of marine, rock and lake origin; Carbon dioxide and Green house gases, Chloralkali Industry, Cement and Concrete Products; Fuel Cells;; Extractive metallurgy; Solid State Technologies, Sol-Gel, Magnetic materials and Superconductors; Materials for electronics

**BOOKS RECOMMENDED**

1. Cotton FA, Wilkinson G, Murillo CA and Bochmann M "Advanced Inorganic Chemistry" 2<sup>nd</sup> Ed (1987) John Wiley and Sons, Inc
2. Cotton FA, Wilkinson G, Murillo CA and Bochmann M "Basic Inorganic Chemistry" 2<sup>nd</sup> Ed (1987) John Wiley and Sons, Inc
3. Bochmann M "Organometallics: Complexes with Transition Metal-Carbon  $\sigma$ -Bond" (1994) Oxford University Publications
4. Basolo F and Johnson RC "Coordination Chemistry: The Chemistry of Metal Complexes" (1964) W. A. Benjamin, Inc
5. Swaddle TW "Inorganic Chemistry: An Industrial and Environmental Perspective" (1997) Academic Press
6. Buchner W, Schliebs R and Winter G "Industrial Inorganic Chemistry" (1989) KH Buchel
7. Buchel KH, Moretto HH and Woditsch P "Industrial Inorganic Chemistry" 2<sup>nd</sup> Ed (2000) Wiley-VCH

**CHM-638: BIOINORGANIC CHEMISTRY**

Credit Hours: (3+0)

Development and Importance of Bio-Inorganic Chemistry, Introduction to Metals of Biological Importance, Role of Different Metals in Biological System, Metal Deficiencies and Metal Overload in Biological System, Metalloproteins: Transferrin and Ferritin, Iron Sulphur Proteins, Iron Transport Mechanism, Protein Peptides, Metallo-enzymes and Metal activated enzymes, Carbonic anhydrase, Carboxy Peptidase, Alkaline Phosphatase, Chlorin and Porphyrin Metal Complexes, Cytochrome, Myoglobin and Haemoglobin, Haemocyanin, Vitamin B<sub>12</sub>, Oxygen carriers, Nitrogen Fixation, Chelation Therapy and Metallotherapy Photosynthesis.

#### **BOOKS RECOMMENDED**

1. Hay RW "Bio-inorganic Chemistry" (1987) Ellis Horwood Limited
2. Lippard S J and Berg JM "Principles of Bioinorganic Chemistry" University Science Books
3. Das AK "A Text book on Medicinal Aspects of Bio-Inorganic Chemistry" (1909) CBS Publishers and Distributors
4. Cox PA "The Elements on Earth: Inorganic Chemistry in the Environment" (1995) Oxford University Press
5. Hay RW "Bio-inorganic Chemistry" Ellis Harwood Limited (1987)
6. Lippard SJ and Berg JM "Principles of Bioinorganic Chemistry" (1994) University Science Books

#### **CHM-648: SYNTHESIS, ANALYSIS AND CHARACTERIZATION OF TRANSITION METAL COMPLEXES**

Credit Hours: (0+3)

1. Synthesis and characterization of  $K_3[Fe(ox)_3] \cdot 3H_2O$ ,  $[Co(phen)_3]Br_2$ ,  $trans-[Co(en)_2 Cl_2]$  and  $cis-[Co(en)_2 Cl_2]$ ,  $NH_4[Cr(NH_3)_2(NCS)_4] \cdot xH_2O$ ,  $[Co(NH_3)_5Cl]Cl_2$ ,  $[Co(NH_3)_5ONO]Cl_2$  and  $[Co(NH_3)_5NO_2]Cl_2$
2. Ion exchange separation of chromium complexes.

### **BOOKS RECOMMENDED**

1. Adams DM and Raynor JB "Advanced Practical Inorganic Chemistry" (1965) John Wiley and Sons, Ltd
2. Pass G and Sutcliffe H "Practical Inorganic Chemistry" 2<sup>nd</sup> Ed (1974) Chapman and Hall Ltd
3. Girolami GS, Rauchfuss TB and Angelici RJ "Synthesis and Techniques in Inorganic Chemistry: A Laboratory Manual" 3<sup>rd</sup> Ed University Science Books Sausalito, CA
4. Woollins JD "Inorganic Experiments" (1994) VCH Publisher, Inc
5. Shriver DF, Atkins PW and Langford CH "Inorganic Chemistry" (1994) Oxford University Press
6. Vogel AI "A Textbook of Inorganic Quantitative Analysis" (1987) Longman.

### **CHM-658: ANALYSIS OF REAL SAMPLES USING STATISTICAL METHODS**

Credit Hours: (0+3)

The laboratory course is based on the analysis of real samples using mainly titrimetric and gravimetric methods of analysis. The techniques include neutralization titrations, redox titrations, complexometry, ion-exchange chromatography and gravimetry. Accuracy and precision of results will be checked using different statistical and computational methods by performing experiments using more than one method.

Analysis of Acetic Acid in Vinegar, Calcium in Eggshell by Back Titration, Calcium in Milk by EDTA Back-Titration, Mixture of  $Mg^{+2}$  and  $Mn^{+2}$  by EDTA, Copper by Iodometry, Copper by Complexometric Titration, Magnesium Hydroxide in Milk of Magnesia, Ascorbic Acid in Vitamin Tablets, Sodium Hypochlorite in Commercial Bleach by Iodometry, Temporary and Permanent Hardness of Water, Total Cations in Water by Cation Exchange Chromatography, Copper as  $CuO$  by Gravimetry, Separation of Two Cations by Anion Exchange Chromatography. Homogenous Precipitation of Fe as  $Fe_2O_3$ .

### **BOOKS RECOMMENDED**

1. Marr G and Rockett BW "Practical Inorganic Chemistry" (1972) Van Nostrand Reinhold Company

2. Reif F "Statistical Physics-Berkeley Physics Course" (1965 )New York McGraw Hill
3. Grant GH and Richard WG "Computational Chemistry" Oxford Science Publications
4. Vogel AI "A Textbook of Inorganic Quantitative Analysis" (1987) Longman

### **CHM-638.1: INDUSTRIAL ENVIRONMENTAL CHEMISTRY**

Credit Hours: (3+0)

#### **Optional Course Offered in lieu of CHM-638**

Review of Basic Chemical Principles and Nomenclature; Introduction to Environmental Chemistry with a Discussion of Elemental Cycles.

Aquatic Chemistry: Metal Ions, and Suspensions; Complexation and Chelation; Common Pollutants (Agricultural and Biological Interactions); Redox Chemistry in Aqueous Systems and pE; Solubility (Equilibrium, States, Aqueous Interactions, etc.); Colloidal Particle Formation and Related Interactions; Heavy Metal and Other Contributions to Pollution (including Pesticides); Role of Halogenated Hydrocarbons in Pollution; Water Pollution and Treatment from a Chemical Standpoint; Interactions with Atmosphere, Soil, and Other Interfaces. Geospheric Chemistry: Soil Chemistry; Ion-Exchange; Acidity and Basicity in Soil; Transport and Interactions; Chemical Interaction; Participation in Cycles. Atmospheric Chemistry: Significance, Physical and Chemical Make-up, and Characteristics; Chemical Interactions in the Atmosphere; Photochemistry, Atmospheric Cycles S, N, O, C, X (Halogen) and other Specific Interactions; Particulate Composition, Chemistry, Transport, and Reactions; Significance of Emissions; Ozone Degradation. Tangential Subjects: Speciation of Environmental Components; Significance of Elemental Species; Detection of Species; Measurement of Species. Special Topics: Anthropogenic Identification by Application of Modern Statistical Tools.

Quality Control (QC) and Quality Assurance (QA); Quality Control Methods: Environmental Quality Management System ISO 14000; Requirements, Conformances, Non Conformance; Audits and Audit Stages; Role and Responsibilities of Lead Auditor, Detection-Prevention and Waste Minimization, Industrial Environmental Problems; ISO 9000 and Other Specific ISO Methods.

## BOOKS RECOMMENDED

1. Swaddle TW "Inorganic Chemistry: An Industrial and Environmental Perspective" (1997) Academic Press
2. Buchner W, Schliebs R and Winter G "Industrial Inorganic Chemistry" (1989) KH Buchel
3. Buchel KH, Moretto HH and Woditsch P "Industrial Inorganic Chemistry" 2<sup>nd</sup> Ed (2000) Wiley-VCH
4. Manahan SE "Environmental Chemistry" 7<sup>th</sup> Ed (2004) CRC Press; New York
5. Gianguzza A, Pelizzetti E and Sammartano S "Marine Chemistry: An Environmental Analytical Chemistry Approach" (1997) Springer
6. Howard G "Aquatic Environmental Chemistry" (1998) Oxford University Press, USA
7. Sparks DL "Environmental Soil Chemistry" 2<sup>nd</sup> Ed (2002) Academic Press
8. Cresser M, Killham K, Edwards A, Campbell PGC, Harrison RM and De Mora SJ "Soil Chemistry and its Applications" (1993) Cambridge University Press
9. Dragun J "Soil Chemistry of Hazardous Materials" (1988) Hazardous Materials Control
10. Goetsch DL and Davis SB "ISO 14000: Environmental Management" 1<sup>st</sup> Ed (2000) Prentice Hall
11. Gitlow HS "Quality Management Systems: A Practical Guide" (2000) CRC Press.

## **ORGANIC CHEMISTRY**

### **SEMESTER- VII**

#### **CHM-613: SPECTROSCOPIC STUDIES OF ORGANIC MOLECULES**

Credit Hours (3+0)

#### **BASIC**

Energy and electromagnetic spectrum, Units, Absorption of electromagnetic radiations by organic molecules, Atoms and molecules absorb light of certain wavelength, Understanding the origin of vibrational, rotational and electronic spectra. Determination of the

energy difference between rotational, vibrational and electronic energy levels of molecules.

### **INFRARED SPECTROSCOPY: BASIC CONCEPTS**

Applications, Bond Properties and absorption mechanism, Instrumentation-I.R. Spectrometer, FT-IR, Sampling, Distinction between two different functional group isomers by I.R, Distinction between position isomers of alkenes, alkynes and derivatives of benzene, Interpretation of spectra, Factors affecting the absorption frequency of various functional groups: Conjugation effect, Ring size effect with internal double bond and external double bond, Hybridization effect and substituent effect, Stretching vibration frequency of carbonyl group in ketone, aldehyde, carboxylic acids, esters, amides, acid chlorides, anhydride, amine, nitrile and imines, sulphur, phosphorus compounds and problems.

### **<sup>1</sup>H-NMR-NUCLEAR MAGNETIC RESONANCE**

Chemical shifts; factors affecting chemical shifts. Spin-spin coupling, Coupling Constants; Mechanism of coupling, One bond coupling (<sup>1</sup>J), Two bond coupling (<sup>2</sup>J)(Gem Vicinal Coupling), Three bond coupling (<sup>3</sup>J-Vicinal Coupling), Long Range coupling, Magnetic Equivalence, Failure of N+1 Rule, Mechanism of coupling in alkenes (Allylic Coupling), Protons on alcohols and nitrogen, Spin system notation (A<sub>2</sub>, AB and AX spin System, AB<sub>2</sub>, ----AX<sub>2</sub> and A<sub>2</sub>B<sub>2</sub>...A<sub>2</sub>X<sub>2</sub> spin systems), Homotopic, Enantiotopic and Diastereotopic system, Spin-spin-decoupling method.

Pulsed Fourier Transform NMR Spectroscopy: Sensitivity, Rotating frame of Reference, Free Induction Decay, Setting Pulse Width, Adjustment of Pulse Frequency, Phase Corrections, Double Resonance, Off-Resonance Decoupling.

### **CARBON-13-NMR INTRODUCTION**

<sup>13</sup>C-Nucleus, Interpretation of <sup>13</sup>C Spectra (Peak assignment), Chemical Shifts, Calculations of <sup>13</sup>C Chemical shifts, Proton-coupled <sup>13</sup>C-spectra; spin-spin splitting of <sup>13</sup>C, Proton-decoupled <sup>13</sup>C Spectra, NOE (Nuclear-Overhauser-Enhancement), Molecular relaxation process, Sample-spectra-equivalent Carbon, C-13 NMR solvent, Hetero-nuclear coupling of carbon to deuterium and problems (elucidation of structures of organic compounds by <sup>1</sup>H or <sup>13</sup>C-NMR spectra).

### **ULTRA VIOLET SPECTROSCOPY**

Nature of electronic excitation, Principles of absorption spectroscopy, Instrumentations, Chromophores: Effect of conjugation, Woodward

Fieser rules of dienes, Calculations of  $\lambda_{\max}$ ,  $\alpha$ - $\beta$  unsaturated compounds, Substituents with unshared electrons and problems.

### **MASS SPECTROSCOPY**

a. Ionization: Ion Source and Methods of ionization (EI, CI, FI, FD, FAB, Plasma desorption, Laser desorption), SIMS (Secondary Ion Mass Spectroscopy)

b. High Resolution Mass Spectroscopy, Molecular Mass by isotopic atoms

c. GC-Mass Spectroscopy, Instrumentation, Columns Carrier gases, Stationary Phases.

d. LC-Mass Spectroscopy, Instrumentation, Types of Interfaces, Thermal Spray Interface, Moving belt interface, Continuous Flow, FAB Coupling, Electron Spray, Ion Spray.

e. Problems in Mass Spectroscopy.

### **COMBINED STRUCTURAL PROBLEMS BASED ON SPECTRAL DATA**

Minimum 20 problems.

### **BOOKS RECOMMENDED**

1. Pavia.DL, Lampman GL and Kriz GS "Introduction to Spectroscopy: A Guide for students of Organic Chemistry" 3<sup>rd</sup> Ed (2001) Saunders College Publishing/Hott.Rinehart and Winston
2. Silverstein.RM, Bassler GC and Morrill TC "Spectrometric Identification of Organic Compounds" 4<sup>th</sup> Ed (1981)John Wiley and Sons, Inc
3. Kemp W "Organic Spectroscopy" 3<sup>rd</sup> Ed (1991) Macmillan Education Ltd
4. Whittaker D "Interpretation Organic Spectra" (2000) The Royal Society of Chemistry

### **CHM-623: ADVANCED ORGANIC REACTION MECHANISM (PART-1)**

Credit Hours: (3+0)

### **NUCLEOPHILIC SUBSTITUTION REACTIONS**

Introduction to Nucleophilic substitution reactions, Methods of determining reaction mechanism: Kinetics methods; Collision theory

and transition state theory Chemical methods; Study of products, Study of intermediates, trapping of intermediates, Stereo chemical studies, Isotopic labeling, Kinetic isotopic effects (primary and secondary), Crossover experiments, Hammett equation, thermodynamic and kinetic control.

### **NUCLEOPHILIC SUBSTITUTION REACTIONS AT SATURATED CARBONS**

$S_N^1$  and  $S_N^2$  reactions: kinetics and characteristics, Mass law effect, Salt effect, effect of solvents, Nucleophiles, Leaving groups, Substituents at  $\alpha$  and  $\beta$  carbons on  $S_N^1$  and  $S_N^2$  reactions. Ion pair mechanism and  $S_N^1$  reactions, Borderline cases and allylic rearrangements, Neighboring group participation; Neighboring group participation of electron rich groups, Neighboring group participation by double bonds, Aromatic rings and O bonds.  $S_N^1$  and  $S_N^2$  and  $S_N^1$  mechanisms.

### **NUCLEOPHILIC SUBSTITUTION REACTIONS AT UNSATURATED**

Nucleophilic substitution reactions at carbon-carbon double bond, Nucleophilic substitution reaction and carbon-oxygen double bond: reactivity, reactions and mechanism of acid derivatives with alcohols, Water and amines, Chemistry of carbenes ; Structure and reactivity Formations and reactions.

### **EXAMPLES OF NUCLEOPHILIC SUBSTITUTION REACTIONS**

Reactions of carbon nucleophiles: Organometallic compounds; Formation and reactions of Grignard reagent, Organosodium and potassium compounds, Organocopper compounds and acetylides. Enols and enolates and their equivalents; Formation and reactions ( alkylation, acylation, halogenation and nitrosation) of enols and enolates. Thermodynamically and kinetically stable enolates and their reactions. Scope and limitations of Claisen Ester condensation, Dieckman reaction and throppe reaction, Reactions of oxygen nucleophiles: Williamson's synthesis. Reaction of nitrogen nucleophiles: reactions of amines, Gabriel's synthesis.

### **NUCLEOPHILIC SUBSTITUTIONS ANSMAHI**

$S_NAr$ , Benzynes  $S_N1$  and  $S_N1$  mechanisms  
Aliphatic Electrophilic substitution reactions  
 $S_E1$ ,  $S_E2$  and  $S_Ei$  reactions Examples

### **ELECTROPHILIC AROMATIC SUBSTITUTION REACTIONS**

Reactivity of benzene, polynuclear aromatic hydrocarbons and heterocyclic compounds (Pyrrole, Furan, Thiophene and Pyridine) Reactions and their mechanism- A comparative study of reagents and reactions conditions of nitration, halogenation, sulphonation, alkylation, acylation and nitrosation of benzene, polynuclear hydrocarbons and heterocyclic compounds.

Examples of electrophilic aromatic substitution reactions, their mechanism, scope and limitations: Sandmeyer reaction, Gatterman reaction, Gatterman- Koch reaction, Houben and Hoesch reaction, Kolbe-Schmidt reaction, Riemer-Tiemann reaction, Vilsmeier reaction, Diazocoupling reaction, Ullmann reaction, Ritter reaction.

### **BOOKS RECOMMENDED**

1. Sykes P "A Guide Book to Mechanism in Organic Chemistry" (1986) Longman
2. Gould ES "Mechanism and Structure of Organic Chemistry" (1959) Holt, Rinehart and Winston Inc
3. March J "Advanced Organic chemistry Reactions, Mechanisms and Structures" 4<sup>th</sup> Ed (1992) John Wiley and Sons Inc
4. Cleyden J, Greeves N, Warren S and Wothers P "Organic Chemistry" (2001) Oxford University Press

### **CHM-633: PHARMACEUTICAL CHEMISTRY**

Credit Hours: (3+0)

**A:** How chemical become drugs. How drugs act & why?

- 1 Physicochemical Properties in Relation to Biological Action. Complex events between drug administration and drug action. Solubility and partition coefficient. Drug-Receptor interactions.
- 2 Factors influencing dosage formulations. Disintegration & dissolution. Absorption of drugs, its pre-requisites, effective blood level, Placebo effects, MIC values etc. Drug-drug interactions
- 3 Drug Metabolism Factors influencing metabolism of drugs. Site of metabolism, metabolic changes in GI tract. Types of metabolic reactions. Reactions based on functional group.
- 4 Structure-Activity Relationship (SAR) Chemical Structure in relation to Biological activity of molecules. Stereochemical factors in SAR. Effect of various functional groups on the biological activity of molecules. Prodrugs, Isosters and Pharmacophore groups.

**B:** Synthesis, Physical & Chemical Properties, Mode of action, SAR studies and Toxicity of:

- 1 Sulfa drugs. Sulfa drugs in current therapy (Human and Veterinary Veterinary use).
- 2 Drugs acting on NIDDM. Sulfonyleureas.
- 3 Antibiotics. Penicillins, cephalosporins, tetracyclines, chloramphenicol, quinolones.
- 4 Anti-viral agents and anti-neoplastic agents.
- 5 Histamines and antihistamines. H<sub>1</sub> and H<sub>2</sub>-receptor antagonists. Proton pump inhibitors.
- 6 Antimalarials
- 7 Analgesics. (Peripheral as well as centrally acting)
- 8 Local Anaesthetics

**C:** Recent trends in drug development. Quantitative structure activity relationship (QSAR), Computer Models & simulations with examples (Case study of at least one drug).

### **BOOKS RECOMMENDED**

1. Burger A "Medicinal Chemistry" 4<sup>th</sup> and 5<sup>th</sup> Ed Wiley Interscience
2. Gisvold W and Doerge "A Text Book of Organic Medicinal and Pharmaceutical Chemistry" 9<sup>th</sup> Ed Lippincott
3. Korolkovas and Burckhaliter "Essentials of Medicinal Chemistry" Wiley Interscience New York
4. Jenkins GL et al "The Chemistry of Organic Medicinal Products" Wiley Interscience New York
5. Clarks ECG "Isolation and Identification of Drugs" Vol I and II The Pharmaceutical Press, London

### **CHM-643: QUANTITATIVE ORGANIC ANALYSIS**

Credit Hours: (0+3)

#### **A: DETERMINATION AND ESTIMATION OF SELECTED ELEMENTS IN ORGANIC COMPOUNDS BY GRAVIMETRIC METHOD.**

- 1 To estimate the percentage of sulfur.
- 2 To estimate the percentage of chloride.
- 3 To estimate the percentage of bromide.
- 4 To estimate the percentage of iodide.

#### **B: ESTIMATION OF NITROGEN THROUGH MICRO KJALDAHL METHOD.**

**C: TO ESTIMATE THE FOLLOWING.**

- 1 Estimation of phenols by bromination method.
- 2 Estimation of -NH<sub>2</sub> by acetylation method.
- 3 Estimation of -OH by acetylation method.
- 4 Percentage of amide group in the given organic sample.
5. Percentage and equivalent weight of unknown organic acids (2-3 samples).
6. Est. of ascorbic acid from given samples by oxidation method
7. Determination of steroids by UV spectrophotometric method.
8. Estimation of non-steroidal anti-inflammatory drugs (NSAID's) by UV spectrophotometric method.
9. Estimation of erythromycin by spectrophotometric method.
10. Determination of percentage of glucose by spectrophotometric (o- toluidine) method.
11. Determination and estimation of -OH group in phenols by spectrophotometric method.
12. Percentage of cholesterol in unknown samples by spectrophotometric method.

#### **BOOKS RECOMMENDED**

1. Vogel AI "Quantitative Organic Analysis: Elementary Practical Organic Chemistry part II"
2. Vogel AI "Quantitative Inorganic Analysis" (2000) ELBS
3. Casey M, Leonard J and Lygo B "Advanced Practical Organic Chemistry" (1990) Blackie, Chapman and Hall New York

#### **CHM-653: NATURAL PRODUCTS LABORATORY**

Credit Hours: (0+3)

#### **LITERATURE SURVEY PRESENTATIONS (ORAL AND WRITTEN)**

#### **PRACTICALS PERFORMANCE**

1. Isolation and Identification of caffeine from tea leaves (using M.P, TLC and HPLC).
2. Isolation and Identification of piperine from black pepper (using M.P and TLC).
3. Isolation, identification and hydrolysis of casein from milk (chemical tests and paper chromatography of amino acids).
4. Isolation and Identification of cystine from human hair (using paper chromatography and chemical tests).
5. Isolation of phosphates from milk.

6. Isolation and Identification of lactose from milk (using TLC, paper chromatography and chemical tests).
7. Isolation and Identification of glucose from cane sugar (using TLC, paper chromatography and chemical tests).
8. Isolation and Identification of starch from potato (using chemical tests).
9. Isolation and Identification of mucic acid from milk.
10. Isolation and Identification of friedelin from cork (using HPLC).
11. Molecular modeling studies of friedelinol and epi-friedelin.
12. Isolation and Identification of azelaic acid from castor oil (using Gas chromatography).
13. Isolation of stigmasterol from soya beans.
14. Isolation and Identification (using UV-spectroscopy studies to elaborate substitution pattern in flavinoids) of naringin from grape fruit.
15. Isolation and Identification of hesperidine from orange peels (using UV-spectroscopic studies).
16. Isolation and column chromatography of pigments from spinach.
17. Isolation and Identification (using GCMS) of limonene and other volatile compounds of orange peels by steam distillation.

#### **BOOKS RECOMMENDED**

1. Ikan R "A Laboratory Guide" (1969) Academic Press
2. Harbon TB "Phytochemical Methods" A Guide to Modern Techniques of Plant Analysis 2<sup>nd</sup> and 3<sup>rd</sup> Ed (1988) Chapman

#### **CHM 633.1: ADVANCED CHEMISTRY OF ALKALOIDS**

Credit Hours: (0+3)

Introduction, Occurrence, Classification, Nomenclature, Physical and Chemical properties. Detection, isolation and purification techniques. Pharmacological importance of alkaloids. Biosynthesis of vinblastine, ajmaline, jervine, imperialine and solanidine. Biosynthesis of ajmaline and jervine. Structure elucidation and Stereochemistry of following groups of alkaloids by modern spectroscopic techniques (UV, IR, Mass <sup>1</sup>H NMR, <sup>13</sup>C NMR, COSY, HMQC, HMBC, HOHAHA, NOESY)

a) Buxus, b) Veratrum, c) Indole, d) Diterpenoidal alkaloids

#### **BOOKS RECOMMENDED**

1. "The alkaloids Specialist Periodical Reports (All Volumes )" The Chemical Society London
2. Manske "The Alkaloids" (Vol 1-33) Academic Press

3. Rehman A and Basha A "The Biogenesis Indole Alkaloids"  
(1982) Oxford university press England
4. Cordell GA "Introduction to Alkaloids a Biogenetic Approach"  
(1981) Wiley Inter Science Publications

**CHM 633.2: CHEMISTRY OF ORGANIC NITROGEN  
COMPOUNDS EXCULUDING ALKALOIDS**

Credit Hours: (0+3)(OPTIONAL COURSE OFFERED IN LIEU OF CHM-633)

1. Derivatives of Ammonala.
2. Nitramines and Nitramides.
3. Amino Acids. Proteins, Peptides and Enzymes.
4. Aryl Nitrogen Compounds.
5. Dyes, Pigments and color photography.
  - a) Methods for applying Dyes to Fibers.
  - b) Commercial uses of Light Absorbing Compounds.
  - c) Color Photography.
6. Polymers.

**BOOKS RECOMMENDED**

1. Smith PAS "Open Chain Nitrogen Compounds" Benjamin Inc
2. Roberts and Caserio "Principles of Organic Chemistry"

**SEMESTER- VIII**

**CHM-614: ADVANCED ORGANIC REACTIONS**

**Credit Hours (3+0)**

**REACTIONS OF ORGANIC COMPOUNDS AS ACIDS AND  
BASES**

Bronsted theory and Lewis theory of acids and bases, Strength of acids and conjugate acids of

bases and Pka scales, Leveling effect of water. Rate of acid base reactions using the table of Pka values to predict equilibrium in chemical reactions, Pka values, The equilibrium constants and free energy change in reaction, The effect of structural change on acidity, Effect of the atom bonded to hydrogen, Influence of inductive effect, Influence of resonance effect, Effect of hydrogen bonding, Effect of hybridization, Influence of solvent on the strength of acids, Carbon, Nitrogen, Sulphur and halogen acids, General and specific acid base catalysis, Differentiation between nucleophilicity and basicity and acid base indicators (including spectroscopic indicators).

#### **MOLECULAR REARRANGEMENT**

Rearrangement of electron deficient system, Hofmann rearrangement, Curtius and Lossen rearrangement, Beckmann rearrangement, Baeyer rearrangement, Dakin rearrangement, Schmidt rearrangement, Rearrangement of peroxides, Pinacol rearrangement, Wagner Meerwein rearrangement, Wolff rearrangement and Arndt-Eistert synthesis, Rearrangement of electron rich system, Steven's rearrangement, Wittig rearrangement, Sommelet rearrangement, Favorskii rearrangement, Neber rearrangement, Benzil-benzilic acid rearrangement, Allylic rearrangement, Neopentyl rearrangement and Willgerodt reaction.

#### **OXIDATION AND REDUCTION**

Oxidation of common functional groups their procedures and mechanisms, Oxidation by peroxides and hydrogen peroxide, Oxidation by  $\text{KMnO}_4$  and osmium tetroxide, Oxidation by Iodine-Silver acetate reagent, Ozonolysis, Oxidation by Chromium (IV) oxide and with chromyl chloride, Oxidation by nitric acid, Oxidation by selenium oxide, Catalytic dehydrogenation, Reduction of common functional groups and their mechanism, Reduction by

addition of electron, Reduction by hydride transfer and reduction by catalyzed addition of molecular hydrogen.

#### **PHOTOCHEMICAL REACTIONS**

Principle of photochemical reactions, Photochemical reductions, Photochemical addition, Photoaddition of alkenes to carbonyl compounds, Photoaddition of alkenes and alkynes to aromatic compounds, Photodimerisation of alkenes, conjugated dienes and aromatic compounds, Photorearrangement, Cis trans isomerisation, Intramolecular photocyclisation, Conjugated dienes, Cage compounds, Sigmatropic rearrangement, Cyclohexadienone, Photodimerisation of benzenoid compounds, Photooxidation, Formation of peroxy compounds, Oxidative coupling of aromatic compounds, Photolysis of carbonyl compounds, Photolysis of compounds containing the  $\text{N}^+=\text{N}^-$  group, Diazotization & alkylazides.

#### **THE CHEMISTRY OF RADICALS**

Introduction to the reaction of radicals, Comparison of the geometry and stability of radicals, cations and anions, Methods of generating radicals, Thermal cleavage, Photochemical cleavage from other radical reaction. Redox reaction. Stable free radicals; factors influencing reactivity and stability of radicals. The general radical reactions, Radical coupling and disproportionation, Abstraction reaction involving sigma bond. Addition of radical to common unsaturated grouping, Radical chain reactions, Rearrangements, Formation of carbon-halogen bond, Substitution in saturated compounds, Substitution in allylic and benzylic compounds, the use of (NBS), Addition to carbon multiple bonds, Bromodecarboxylation, Iododecarboxylation, Formation of carbon-carbon bond, By addition to carbon-carbon double bond,

By intramolecular addition reaction, By alkenyl and aryl addition, By polymerization of alkenes, By homolytic aromatic substitution, Dimerization of alkyl radical: The Kolbi electrolytic reaction, Dimerization of aryl radicals: The Ullmann reaction, Pinacol reaction, A radical dimerisation, The acylion synthesis, Formation of carbon-nitrogen bond, Nitration at saturated carbon, By addition to carbon multiple bonds, Autoxidation, Oxidation of phenols, Oxidative coupling of phenols, Phenols, Vitamin E & K as antioxidants, Reduction and radical anions, Vinyl polymerization and Biradicals.

6. Synthesis and reactions of following heterocyclics
  - a) Non aromatic heterocyclic compounds containing N, O & S i.e., Dioxane, Pyrrolidine, Aziridine etc.
  - b) Aromatic heterocyclic compounds, Pyrrole, thiophane etc
  - c. Condensed aromatic heterocyclic compounds

#### **BOOKS RECOMMENDED**

1. March J "Advanced Organic Chemistry Reactions, Mechanism and Structure" 4<sup>th</sup> Ed (1992) John Wiley and Sons Inc
2. Sykes P "A Guide Book to Mechanism in Organic Chemistry" (1986) Longman group Ltd.
3. Cleyden J, Greeves N, Warren S and Wothers P "Organic Chemistry" (2001) Oxford University Press.
4. Parkimns AW and RC Poller "An Introduction to Organometallic chemistry" (1986) Mac Millan Publishers, HongKong
5. Powell P "Principles of Organometallic Chemistry" (1988) Chapman and Hall, London.
6. Pearson AJ "Metallo-organic Chemistry" (1985) John Wiley, New York

#### **CHM-624: ADVANCED ORGANIC REACTION MECHANISM PART- II**

Credit Hours (3+0)

#### **ELECTROPHILIC & NUCLEOPHILIC ADDITION TO CARBON-CARBON DOUBLE BONDS**

Addition of halogens: Mechanism (ANTI & SYN), Effect of substituents on rate of addition, Orientation of addition, Addition of unsymmetrical reagents (Addition of halogen derivatives, Hydration, carbocations, Hydroxylation). Addition Of symmetrical reagents (Hydrogenation, Ozonolysis), Addition to conjugated dienes (1,2 & 1,4-addition, Diels-Alder reaction), Nucleophilic addition (Cyanoethylation, Michael reaction). Oxymercuration and demercuration, hydroboration etc. Regioselectivity, regioselectivity and stereochemical aspects of addition products.

### **NUCLEOPHILIC ADDITION TO CARBON-OXYGEN DOUBLE BONDS**

Electrophilic and nucleophilic reactivity of carbon-oxygen double bond. Simple addition reactions: (Addition of water-Hydration, Addition of alcohol, Addition of thiol, Addition of Hydrogen cyanide, Addition of Bisulphate, Addition of hydride ions: Metal hydride ions, Meerwein-Ponndorf reaction, Cannizzaro reaction; Addition-elimination reactions: Derivatives of ammonia; Carbon as Nucleophile. Grignard reagent, Acetylide anions, Aldol reactions, Nitroalkanes Perkin reaction, Knoevenagel & Stobbe reactions, Benzoin condensation, Leukart reaction, Strecker synthesis. Nucleophilic addition to carbonyl analogues. Stereo selectivity in carbonyl addition reaction: Cram's Rule.

### **MOLECULAR ORBITAL & ORGANIC REACTIONS**

Pericyclic reactions, Frontier orbital theory. General description of the Diels Alder reactions Dienes, dienophiles "the endo rule for the diels Alder reactions Intermolecular Diels Alder reactions. The Woodward-Hoffmann description of Diels Alder reaction

### **ELIMINATION REACTIONS**

1,2- or  $\beta$ -elimination, E1 mechanism, E1cB mechanism, E2 mechanism: Stereochemistry in E2 mechanism, Orientation in E2 elimination (Saytzev elimination, Hofmann elimination, Bredt's elimination) Elimination vs Substitution, Effect of activating groups, 1,1- ( $\alpha$ ) elimination, Pyrolytic elimination (Chugaev reaction, Cope reaction).

### **CHEMISTRY OF ORGANOMETALLIC COMPOUNDS**

Structure and bonding in transition and non-transition metal compounds and complexes. Donor vs acceptor ligands and their effect on the central metal atom. 16 and 18 electron complexes. Complexes of organic functionalities, olefins, acetylenes, alkenes and their reactivities. Oxidative additions and reductive eliminations.

Applications of organometallic compounds using Cu, Pd, Co, Fe, Ni, W, Zn in organic synthesis: hydrogenation, isomerisation, coupling, cyclisation, cycloaddition, carbonylation rearrangements.

### **BOOKS RECOMMENDED**

1. Lowry TH and Richardson K.S “Mechanism and theory in Organic Chemistry” (1976) Harper and Row
2. Sykes P “A Guide Book to Mechanism in Organic Chemistry” (1986) Longman
3. Gould ES “Mechanism and Structure of Organic Chemistry” (1959) Holt, Rinehart and Winston Inc
4. Streitwieser A and Heathcock CH “Introduction to Organic Chemistry” 3<sup>rd</sup> Ed (1989) Macmillan Publishing Company
5. March J “Advanced Organic Chemistry Reactions, Mechanisms and Structures” 4<sup>th</sup> Ed (1992) John Wiley and Sons Inc
6. Den G, Warren and Wothers “Organic Chemistry” (2001) Oxford University Press

### **CHM-634: STEREOCHEMISTRY**

Credit Hours: (3+0)

#### **INTRODUCTION:**

Different models and conventions for drawing three dimensional structures: Drawing of Flying Wedge, Fischer Projection, Newman Projection and Sawhorse Conventions.

Difference between Configuration and Conformation. Concept of rotation about single bonds and restricted rotation about double bond in view of symmetry of electron densities of molecular orbital for  $\sigma$  and  $\pi$  bonds.

#### **MOLECULAR SYMMETRY AND CHIRALITY:**

Symmetry operations and Symmetry elements; axis, plane or centre. Point group classification: (i)  $C_1$  Chirality: chirotopicity and stereogenicity. Molecules with one stereogenic or chiral center. Enantiomers and racemic mixture and R and S nomenclature of a chiral centre. Plane polarized light and optical activity. Polarimeter and specific rotation. Description of enantiomers as (+) or (-) and D or L. Absolute and relative stereochemistry. Molecules with more than one

stereogenic center: Diastereoisomers with more than one stereogenic centre. Diastereoisomers. Conversion of enantiomers and diastereoisomers. Achiral compounds with more than one stereogenic centre. Constitutionally unsymmetrical chiral molecules; erythro and threo. Re and Si faces. Constitutionally symmetrical chiral molecules. Diastereoisomerism E and Z nomenclature for compounds with more than one non-cumulated double bonds. (ii) Axial and Planar Chirality: In appropriately substituted alkenes, alkyldiene, cycloalkanes, spirans, adamantoids, biaryl, trans cycloalkenes and cyclophanes.

#### **TOPICITY AND PROSTEREOMERISM:**

Topicity of Ligands: Homotopic, enantiotopic, diastereotopic ligands and faces. Stereoheterotopic ligands and faces; Molecules with one prochiral centre and pro-pseudosymmetrical centre. Molecules with more than one prochiral centre. Molecules with a chiral as well as prochiral centre. Molecules with a prochiral axis; Molecules with a prochiral plane. Molecules with prostereogenic prochiral centres. Re and Si system of nomenclature for ligands. Stereoheterotropic ligands and NMR spectroscopy. Chemical and biochemical transformation of heterotropic ligands and faces.

#### **RACEMISATION AND RESOLUTION:**

Racemisation: Involving carbocations, carbanions, free radicals, stable symmetrical intermediates through rotation about bond, configurational change in substitution reactions. Asymmetric transformation and metarotation. Resolution: Methods of resolution through mechanical separation, formation of diastereoisomeric salts, formation of molecular complexes, chromatography, kinetic equilibrium, asymmetry transformation, biochemical transformation, inclusion compounds.

#### **OPTICAL PURITY AND ENANTIOMERIC EXCESS:**

Isotopic dilution method, Enzymic methods, gas chromatographic methods and NMR spectroscopic methods (use of diastereoisomers, shift reagents, chiral solvating agents).

#### **CONFORMATIONS OF ACYCLIC SYSTEMS:**

Conformations of ethane, butane, haloalkane, n-propylchloride, 1,2-dihalogeno ethanes, 1,2-diols. Conformations about  $sp^3-sp^2$  and  $sp^2-sp^2$  bonds. Diastereoisomers; configuration and conformations;

diastereoisomers with two vicinal halogens, diastereoisomers with two vicinal hydroxyl groups, diastereoisomers with vicinal hydroxyl and amino groups. Klyne-Prelog terminology for torsional angles. Physical methods of conformational analysis; thermodynamic, dipole moment and spectroscopic methods.

#### **CONFORMATIONS OF CYCLIC SYSTEMS:**

Monocyclic compounds (3, 4, 5, 6, 7, 8 or larger membered rings): Baeyer strain, Pitzer (torsional) strain and Stoll strain (nonbonded interactions) in small, normal, medium and large rings. Conformations of 3, 4, 5 membered rings. Conformations of cyclohexane: boat, chair, half chair, twist conformations. Drawing of chair conformations and axial and equatorial bonds. Ring inversion. Conformations of monosubstituted cyclohexanes. Isolation and characterization of conformers. Disubstituted cyclohexanes, cis and trans isomer and their preferences. Reflex effect. Cyclohexane with one or two  $sp^2$  carbons. Conformations of cyclohexene. Conformations of 7 and 8 membered rings. Effect of strain on methods of formation and reactions of different rings. Conformational analysis of heterocycles. Conformation of fused rings. Cis and trans fused decalines. Fused bicyclic rings with nitrogen. Conformations of bicyclo [4.3.0]nonane, bicyclo [3.3.0]octane, bicyclo [3.2.0]heptane. Bridged ring systems: bicyclo [1.1.1]pentane, bicyclo [2.2.1]heptane, bicyclo [2.2.2]octane. Conformations and reactivity.

#### **STEREOSELECTIVE REACTIONS:**

Stereoselectivity, Asymmetric synthesis and asymmetric induction. Acyclic stereoselective addition of nucleophiles to carbonyl compounds, addition of enolates to carbonyl compounds. Selective transformation of C = C bonds. Diastereoselectivity in cyclic systems: nucleophilic addition to cyclic ketones. Enantioselective synthesis.

#### **MOLECULAR DISSYMMETRY AND CHIROPTICAL PROPERTIES:**

Circular birefringences and circular dichroism. ORD and CD curves. Applications of CD and ORD.

#### **BOOKS RECOMMENDED**

1. Giese RW, Mikulak RP and Runquick OA "Stereochemistry: An Introduction A Programmed Text" (1976) Burgess Publishing company, Minnesota

2. Eliel ES, Wilen H and Mandra LN "Stereochemistry of Organic Compounds" (1994) John Wiley and Sons Inc, New York
3. Potapov VW "Stereochemistry" (1979) Mir Publishers, Moscow
4. Nogradi M "Stereoselective Synthesis" (1987) VCH, Weinheim

#### **CHM-644: ORGANIC LABORATORY PREPARATIONS**

Credit Hours: (0+3)

#### **MULTI-STEP SYNTHESIS OF THE FOLLOWING OR SIMILAR OTHER COMPOUNDS**

1. Preparation of sulfanilic acid from aniline.
2. Preparation of methyl orange from sulfanilic acid
3. preparation of benzoic acid and benzyl alcohol from benzaldehyde-Cannizzaro's reaction
4. Preparation of benzanilide from benzoic acid
5. preparation of phthalimide from phthalic anhydride
6. Preparation of phthalamide from phthalimide
7. Preparation of benzpinacolone from benzpinacol
8. Preparation of benzpinacolone from benzpinacol
9. Preparation of diazoaminobenzene from aniline
10. Preparation of *p*-aminoazobenzene from diazoaminobenzene.
11. Preparation of benzophenone oxime from benzophenone
12. Preparation of cinnamic acid from benzaldehyde
13. Preparation of benzilic acid from benzyl
14. Preparation of benzilic acid from benzyl
15. Preparation of *m*-nitroaniline from *m*-dinitrobenzene
16. Preparation of *m*-nitrophenol from *m*-nitroaniline
17. Isomerisation of maleic acid to fumaric acid
18. Preparation of  $\alpha$ -nitronaphthalene from naphthalene
19. Preparation of  $\alpha$ -naphthylamine from  $\alpha$ -nitronaphthalene
20. Preparation of naphthanoic acid from  $\alpha$ -naphthylamine

#### **BOOKS RECOMMENDED**

1. Vogel AI "A Text Book of Organic Practical Chemistry" Longman, (1989) 5<sup>th</sup> Ed
2. S. Gupta and Bajpai, "Experimental Organic Chemistry Basic Techniques and Preparations", Tata McGraw- Hill Publishing Company Limited, New Delhi.
3. G. Mann and C. Saunders, "Practical Organic Chemistry" (1960), Longman, 4<sup>th</sup> Ed

#### **CHM-654: QUALITATIVE ORGANIC ANALYSIS**

Credit Hours: (0+3)

1. Separation of three component mixtures on the basis of their solubilities in the polar and non polar solvents.
2. Identification of individual components of mixture through qualitative tests based on preliminary identification, element tests, functional group tests and physical characteristics etc.
3. Confirmation of components by spectral analysis/ data on the basis of their chemical structures.
4. Derivatisation of identified components.

#### **BOOKS RECOMMENDED**

1. Harwood LM "Experimental Organic Chemistry, Standard and Microscale" 2<sup>nd</sup> Ed (1999) Black Well Science Publishers, London
2. Furniss BS, Hannaford AJ, Smith PWG and Tatchell AR "Vogels Text Book of Practical Organic Chemistry" 5<sup>th</sup> Ed (1989) ELBS Longman
3. Vogel AI "Elementary Practical Organic Chemistry, Qualitative Organic Analysis"
4. Arayne M.S. and Sultana "A manual of Qualitative Organic Analysis" 3<sup>rd</sup> Ed. BCCT, University of Karachi

#### **CHM-634.1: MODERN TRENDS IN ORGANIC SYNTHESIS**

Credit Hours: (3+0)

#### **Optional Course Offered in lieu of CHM-634**

#### **INTRODUCTION TO ORGANIC SYNTHESIS**

The importance of organic synthesis, Bond polarity, Types of organic reactions, Arrow notation. Synthesis of aromatic compounds and sequence of the reactions. Synthesis of aromatic compounds and order of revents

#### **THE BASIC CONCEPTS**

Introduction, Synthetic equivalent to common synthons, Retrosynthetic analysis of a target molecule and its synthesis and solved examples..

#### **DESIGNING OF A SYNTHESIS**

Introduction, Designing of a synthesis, consider a range of possibilities, the availability, starting materials & equipment, Convergent & Linear synthetic approach, Yield & Conversion, Use of Inherent Symmetry, Solved examples.

#### **LATENT POLARITY**

Introduction, Two group disconnection, 1,3,1,5, 1,2, 1,4-difunctionalized compounds and solved examples.

#### **SYNTHESIS OF CYCLIC COMPOUND**

Introduction, Cyclization reactions, Dieckmann Condensation, Micheal Reaction, Annelation, Robinson Annelation, Diels-Alder Annelation, Three membered rings, Epoxide (oxacyclopropanes), Cyclopropanes, Cyclopropyl ketones, Four membered rings, Cyclic ethers, Cyclic amines, Five membered rings, Six membered rings and solved examples.

#### **FUNCTIONAL GROUP INTERCONVERSIONS (FGIS) & PROTECTING GROUPS**

Introduction, Functional group interconversion (FGIs), Carboxylic acid and its derivatives, Aldehydes, Ketones and their derivatives, Alcohols and their derivatives, Oxidation & Reductions, Removal of functional groups, Protecting groups, Protection of alcohols, Acetals, Ethers, Trialkylsilyl ether, Protection of aldehydes and ketones, Protection of amino acids, Protection of sugars and solved examples.

#### **CHEMOSELECTIVITY**

Introduction, Chemoselective reactions, Chemoselective reduction, Chemoselective oxidation, Carbonyl groups, Functional groups of unequal reactivity, Functional groups of equal reactivity and solved examples

#### **REGIOSELECTIVITY**

Introduction, Regioselective preparation of alkenes, Regioselective electrophilic addition to alkenes, Regioselective ring opening of epoxide, Regioselective alkylation of ketones, Regioselective electrophilic aromatic substitution and solved examples

#### **STERESELECTIVITY**

Introduction, Stereospecific reactions, Stereospecificity in  $E_2$  reactions, Stereospecificity in  $SN_2$  reactions, Stereospecificity in hydrogenation, Stereospecificity in hydroxylation, Stereospecificity in Diels-Alder reactions, Stereoselective reactions Stereoselectivity in  $E_2$

reactions, Stereoselective Nucleophilic addition to unsymmetrical ketone and solved examples

#### **BOOKS RECOMMENDED**

1. Warren S "Organic Synthesis The Disconnection Approach" (1982) John Wiley and Sons
2. Norman ROC and Coxon JM "Principle of Organic Synthesis" 3<sup>rd</sup> Ed (1993) Blackie
3. Corey EJ and Cheng XM "The logical of Chemical Synthesis" (1989) Wiley Interscience
4. Greene TW and Nuts PG "Protecting Groups in Organic Synthesis" 2<sup>nd</sup> Ed (1991) John Wiley and Sons
5. Cleyden J, Greeves N, Warren S and Wothers P "Organic Chemistry" Oxford University Press (2001)
6. Nizami SS "Retrosynthetic Approach to Organic Synthesis" (2003), HEC, Islamabad

#### **CHM-634.2: ORGANIC REACTIONS AND MOLECULAR ORBITAL SYMMETRY**

Credit Hours: (3+0)

**Optional Course Offered in lieu of CHM-634**

#### **INTRODUCTION**

Introduction to molecular orbital symmetry (Woodward and Hofmann Rules), Huckel molecular orbitals for ethylene and conjugated polyenes.

Reactions obeying Woodward Hofmann rules.

#### **ELECTROLYTIC REACTIONS:**

##### **a. Frontier Orbital Approach:**

Introduction to frontier orbitals (HOMO and LOMO). Thermal and photochemical conrotatory and disrotatory cyclization of linear  $\Pi$  electrons systems containing 2,4,6 and 8 electrons.

##### **b. Orbital Correction Diagram:**

Introduction. Classification of all the molecular orbitals of reactants and products about a plane and a  $C_2$  axis and building up of an orbital correlation diagram for 2,4,6 and 8  $\Pi$  electrons systems. Stereochemistry of electrocyclic ring opening and closing of electroanalytical reactions (ring opening and ring closure).

Synthetic application of electrocyclic reactions.

### **CYCLOADDITION REACTIONS:**

Introduction. Concepts of suprafacial and antarafacial terminologies.

#### **a. Frontier Orbital Approach:**

Orbital symmetry rule for thermal and photochemical supra-supra, supra-antra, antra-antra cycloaddition of 2+2, 2+4, 4+4  $\pi$  electrons systems and molecular orbital symmetry rules.

#### **b. Orbital Correlation Diagram:**

Classification of molecular orbital for supra-supra, supra-antra, antra-antra cycloaddition of 2+2, 2+4, 4+4  $\pi$  electrons systems and their corresponding products and orbital correlative diagrams. The symmetry rules for thermal cycloaddition reactions. Reactivity, regioselectivity, site selectivity, periselectivity in cycloaddition reactions. Alder's ene reaction. [1,3]-dipolar cycloaddition reactions. Applications of cycloaddition reactions to organic synthesis.

### **SIGMATROPIC REACTIONS:**

#### **a. Migration of Hydrogen:**

Introduction to molecular orbital symmetry rules for thermal and photochemical (suprafacial and antarafacial) [1,2], [1,3], [1,4], [1,5] and [1,7] migration of hydrogen. Examples related to sigmatropic hydrogen migration.

#### **b. Migration of Alkyl Group:**

Stereochemical suprafacial and antarafacial [1,2], [1,3], [1,4], [1,5] and [1,7] migration of an alkyl group. Molecular orbital symmetry rules for alkyl group migration. Examples of Sigmatropic reactions. Applications of Sigmatropic reactions to organic synthesis. Migration of a delocalized system (Cope Rearrangement).

### **SECONDARY EFFECTS IN PERICYCLIC REACTIONS:**

#### **BOOKS RECOMMENDED**

1. Gilchrist TL and Storr RC "Organic Reactions and Orbital Symmetry" (1979) Cambridge University Press, London
2. Giu GB and Willis MR "Pericyclic Reactions" (1974) Chapman and Hall, London
3. Fleming I "Frontier Orbitals and Organic Chemical Reactions" (1982) John Wiley and Sons, London
4. Ansari FL, Qureshi R and Qureshi ML "Electrocyclic Reactions" (1999) Wiley- VCH

5. Halevi EA "Orbital Symmetry and Reaction Mechanism" (1992) Springer Verlagee
6. Woodward RB and Hoffmann R "The Conservation of Orbital Symmetry" (1970) Verlag Chemie, Weinheim

### **CHM-634.3: FOOD AND COSMETIC CHEMISTRY**

1. The chemistry of food components with special reference to processed foods.

#### **FOOD PRESERVATION**

Preservation of Foods containing polar components. Effect of acids, bases and variation in pH etc. Use of NIR in Quality assessments. Preservation of Fat containing foods, like meat, cheese butter margarine etc. Preservation of Dairy Products, Flash heating technique etc.

#### **FOOD COLORS**

The control & use of food colors. Caramels and Beverages

### **COSMETIC CHEMISTRY**

- 1 Introduction to the preparation of skin care & cosmetic products.
- 2 Preparation of Creams, Lotions and Sun-block preparations. Medicated creams. Oil in water & moisturizing preparations. Depletory creams.
- 3 Preparation of Tooth Pastes and Tooth Powders, mouth wash and Gargles.
- 4 Preparation of Hair Dyes, Hair creams, Shampoos, other hair softening and conditioning products.
- 5 Preparation of Health care products; Disinfectants, odour masking products and deodorizers.

#### **SUGGESTED READINGS:**

1. Stille JK "Industrial Organic Chemistry" (1998) Prentice Hall, Inc, Englewood Cliffs, N.J.
2. Coultate TP "Food, The Chemistry of its Components" (2004) Royal Society of Chemistry, London
3. Edwards WP "The Science of Sugar Confectionery" (1996) Royal Society of Chemistry, London
4. Poucher "Perfumes, Cosmetics and Soap" (1990) Vol 1-3 USP

**PHYSICAL CHEMISTRY**  
**SEMESTER VII**

**CHM-615: THERMODYNAMICS & ELECTROCHEMISTRY**

Credit Hours: (3+0)

**PRELIMINARIES**

Entropy, molecular basics of entropy, statistical basis of the second law. Quantum of entropy changes. Third law of thermodynamics.

## **QUANTUM STATES**

Energy levels. Energy compartmentalized into translation, rotation and vibrational segments. Equations for computing these Energies. Microstates, concepts related to occupation of energy states. Boltzmann factor.

## **THE BEHAVIOURS OF HEAT CAPACITY**

Experimental and theoretical discrepancies in recorded heat capacity data. Need for plausible explanation. Advent of quantum theory. Partition function. The relationship of partition function to the various thermodynamic functions.

## **DETERMINATION OF PARTITION FUNCTIONS**

Localized and non localized systems. Partition functions specific to Energy segments. The sackur Tetrode Equation. Equations for Computing Vibrational and Rotational Partition functions. Partition function and equilibrium constants.

## **ELECTROCHEMISTRY**

**Electrical double layer:** Interface, interphase. A look into the interface. OHP and IHP. Contact adsorption Gibbs Surface Excess. Potential differences across metal solution interfaces. Outer and surface potential difference. Galvani potential difference. Electrochemical potential difference. Interfacial tension. Electrocapillary thermodynamics. Lippmann's equation. Helmholtz-perrin model, Gouy-Champmann model. Stern model, and BDM (Bockris-Devanathan-Muller) model. Charge density. Differential capacitance. Shape of capacitance-Charge curve. The Capacitance hump.

## **ELECTRODE KINETICS**

Electrochemical devices. Charge transfer processes in the absence and presence of electrical field. The Over potential. Butler Volmer equation. The Idea of Equilibrium exchange current density. The Symmetry factor. High field and low field approximation. Tafel equation. Nernst equation.

## **BOOKS RECOMMENDED**

1. Gasser RPH and Richards WG "Entropy and Energy Levels"  
(1974) Oxford University Press

2. Wayatt PAH "The Molecular Basis of Entropy and Chemical Equilibrium". (1971) Royal Institute of Chemistry London
3. Smith EB "Basic Chemical Thermodynamics" (1990) 4<sup>th</sup> Ed Oxford University Press
4. Bockris JOM and Reddy AKN "Modern Electrochemistry" Vol I and II, 4<sup>th</sup> Ed (2003) Plenum Press, London
5. Bockris JOM and Drazic D "Electrochemical Science" (1972) Taylor and Francis, London
6. Bockris JOM, Bonciocat N and Gutmann F "An Introduction to Electrochemical Science" (1974) Wykeham Publications, London
7. Bockris JOM and Fredlein RA "A Work Book of Electrochemistry" (1973) Plenum Press, New York
8. Muhammad M and Amjad M "Principles of Electrode Kinetics" (2001) Rooha Printers, Lahore
9. Seddon JM and Gale JD "Thermodynamic and Statistical Mechanics" (2002) Royal Soc Chem, UK

### **CHM-625: POLYMER CHEMISTRY**

Credit Hours: (3+0)

Introduction to Polymers. Step-growth Polymerizations. polymer chain growth. Kinetics of Polymer chain growth. Copolymerization. Emulsion Polymerization. Natural and Inorganic Polymers. Physical Aspects of polymers. Molecular Weights of Polymers: Distributions, averages, and methods of determination. Viscosity. Osmometry. Light scattering method. Diffusion. Sedimentation. Optical rotation method. Structure of Polymer Chain: Introduction to chain isomerism, stereochemistry, configurations, and conformations. (not in Hiemenz). Amorphous State of Polymers: In depth examination of polymer conformation, microstructure, and dynamics in the amorphous state. Polymer viscoelasticity: Stress relaxation, mechanical models of polymer behavior, time-temperature superposition, rheology. Crystalline State of Polymers: Crystallization and kinetics, crystalline structures, experimental methods. Polymer Solutions and Blends: Thermodynamics, phase separation, mechanisms, kinetics. Relaxation and Transitions in Polymers: the glass transition, experimental methods, and introduction to viscoelastic behavior. Mechanical Behavior of Polymers: Polymer fracture, stress-strain behavior, and ultimate properties. Modern Topics of Polymers: Interfaces, Liquid

Crystalline Polymers, Flow-Induced Structures, Use of Polymer in solar cell. Management of Polymer Solid Waste.

#### **BOOKS RECOMMENDED**

1. Hiemenz PC "Polymer Chemistry: The Basic Concepts" (1984) Marcel Dekker
2. Nicholson JW "The chemistry of Polymers" 2<sup>nd</sup> Ed
3. Stevens MP "Polymer Chemistry: An Introduction" (1999) Oxford University Press
4. Allcock HR and Lampe FW "Contemporary Polymer Chemistry" (1990) Prentice-Hall
5. Rudin "The Elements of Polymer Science and Engineering" (1990) Academic Press
6. Sperling LH "Introduction to Physical Polymer Science" (1992) Wiley Interscience
7. Boyd RH and Phillips PJ "The Science of Polymer Molecules" (1993) Cambridge
8. Flory PJ "Principles of Polymer Chemistry" (1953) Cornell

#### **CHM-635: QUANTUM MECHANICS AND SPECTROSCOPY**

Credit Hours: (3+0)

##### **QUANTUM MECHANICS**

Introduction: Classical mechanics and its laws, Max Planck's explanation of black body radiation curves, concept of quantization of energy, quantum theory and Max Planck's quantum theory, de Broglies, postulate and its application. Heisenberg uncertainty principal. Atomic structure: Line spectra of gases the Bohr model, quantization of energy, Bohr radius, and Rydberg constant. Quantum mechanical terms and postulates, eigenfunction, eigenvalue, coordinate systems. Schrodinger wave equation. Particle in a one dimensional and three dimensional box. Hydrogen and hydrogen like ions. The rigid rotor. Lasers, their properties, types and applications.

**SPECTROSCOPY:** Introduction theory of rotational, vibrational, electronic, and molecular systems, Microwave spectroscopy, e.s.r. and e.p.r. spectra, microwave region, rotational line spectra. Linear and asymmetric systems, selection rule, energy and angular momentum, magnetic quantum numbers, summation method, term symbols, instrumentation, nuclear spin, zeeman effect, vibrational spectroscopy, vibrational spectra, Morse curves, rotational fine structures, P branch, R branch and Q branch.

**INFRARED SPECTROSCOPY:** Introduction, theory of molecular vibration, factors influencing vibrational frequencies, sampling

techniques; applications of infrared spectroscopy, identification by finger printing, identification of functional groups.

**NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY:**

Introduction, nuclear spin states, nuclear magnetic moments. Effect of external magnetic field, precessional motion and precessional frequency, energy transition. Chemical environment and number of signal, chemical shift, internal standard. Factors influencing chemical shift. Correction data, choice of solvent, solvent shift, concentration and temperature effects, signal splitting, coupling, constant. Proton nuclear magnetic resonance, spectra of carbocation, carbon-13 NMR (CMR) spectroscopy,

**MASS SPECTROMETRY:** Introduction, experimental, source, analyser, detector, classification of mass analysers, resolution, sensitivity, valley definition, signal to noise ratio, electron impact phenomenon, application of mass spectrometer, ionization/acceleration, ion collection/amplifiers, magnetic field deflection, quadrupole mass spectrometer, double focusing, time of flight.

**BOOKS RECOMMENDED**

1. Chang R "Physical Chemistry with Applications to Biological Systems" 2<sup>nd</sup> Ed (1981)
2. Alberty RA "Physical Chemistry" 7<sup>th</sup> Ed (1987) John Wiley and Sons New York
3. Hanna MW "Quantum Mechanics in Chemistry" 3<sup>rd</sup> Ed (1981) National Book Foundation
4. Cox PA "Introduction to Quantum Theory and Atomic Structure" (1996) Oxford University Press.
5. Banwell CN "Fundamentals of Molecular spectroscopy" Mc FGaw Hill Co, India (1978).
6. Barrow GM "Introduction to Molecular Spectroscopy" (1962) Mc Graw Hill
7. Kemp W "NMR in Chemistry: A Multinuclear Introduction" (1992) The Macmillan Press Ltd
8. Silverstein RM, Terence GCB and Morrill C "Spectrometric Identification of Organic Compounds" (1991) John Wiley and Sons Inc

**CHM-645: pH -METRY AND POTENTIOMETRY LABS**

Credit Hours: (0+3)

### **pH- METRY**

Titration including acid-base neutralization of both strong and weak nature (and mixture of acids)

Detennination of % of a mineral acid in the given vinegar solution

.Detennination of amount of ascorbic acid in a given tablet

.Determination of acetyl salicylic acid in a given tablet

Detennination of folic acid in a given tablet

Detennination of dissociation constants of weak acids using Henderson- Hasselbalch equation

Simultaneous determination of chromate and dichromate in a given sample. Detennination  $K_{sp}$ ,  $\Delta G$ ,  $\Delta S$ , and  $\Delta H$  for the dissolution of calcium hydroxide. Determination of complexation reaction of metals (Cu, Ni, Co) with EDTA Determination of % of  $\text{NaCO}_3$  content in washing soda

### **POTENTIOMETRY**

.Redox titrations using different systems. Standardization of  $\text{KMnO}_4$  by KI. Precipitation and complexation reactions (detennination of halides).

Detennination of  $\text{Fe}^{+2}$  with EDTA, Detennination of Formal potential ( $E^0$ ),  $K_{eq}$  and "n" of some redox systems

### **AMPEROMETRY**

Verification of Randles Sevcik equation for different redox system. Detennination of calibration curve between diffusion current and concentration of analyte. Amperometric titrations of some redox systems

### **BOOKS RECOMMENDED**

1. "Vogels Textbook of Quantitative Inorganic Analysis" 6<sup>th</sup> Ed (1980) ELBS
2. Braun RD "Introduction to Chemical Analysis" (1985) Mc Graw Hill Co
3. Heinemann S "Chemistry Experiments for Instrumental Methods (1987)
4. Harris DC "Quantitative Chemical Analysis" 5<sup>th</sup> Ed (1998) W.H. Freeman and Co, New York
5. Euler WB (2000) J Chemical Education 77 (8) 109

6. Kkalbus LH (1991) J Chemical Education 68(8) 677

### **CHM- 655: SPECTROSCOPY LABS**

Credit Hours: (0+3)

1. Study of the Absorption Spectra of a Conjugated Dye.
2. Determination of the Formula of a Complex ion.
3. Determination of Glucose in Soft drinks.
4. Analysis of Phosphorus in Detergents
5. UV Spectrophotometric determination of Nitrate in Water sample.
6. Quantitative Analysis of Aspirin by Single-Beam and Double-Beam Ultraviolet Absorption Spectrophotometry.
7. Study the effect of auxochromes on the spectrum of the chromophore.
8. Atomic Absorption Analysis of Metals in Cereal.
9. Determination of Anthracene, Benzene and Naphthalene in a mixture by High Performance Liquid Chromatography.
10. Gas Chromatographic determination of water in Acetone, Acetonitrile, Ethanol or Isopropanol.

### **BOOKS RECOMMENDED**

1. Braun RD andWalters F “Applications of Chemical Analysis” (1982)
2. David P “Experiments in Physical Chemistry” 5<sup>th</sup> Ed (1989)
3. Shoemaker CW, Nibler GJW and Christian GD “Analytical Chemistry” 6th Ed (2004)
4. Trost B “Problems in Spectroscopy” (1967)

## **SEMESTER- VIII**

### **CHM- 616: RADIATION CHEMISTRY & PHOTOCHEMISTRY**

Credit Hours: (3+0)

#### **RADIATION CHEMISTRY**

Introduction, history, development and advancement in radiation chemistry. Radiation Sources: Isotope and mechanical sources, pulsed radiolysis and flash spectroscopy. Interaction of Radiation with Matter: Photoelectric and Compton effect, pair production, energy loss, linear energy transfer. RADIATION DOSIMETRY: Dose,

absorbed dose units, radiation yields, dosimetry methods of absolute measurement, chemical dosimetry, Fricke dosimeter, dosimetry in pulse radiolysis. ENERGY STATES IN RADIATION CHEMISTRY: Excited states its production. Product formation through excited state, fragmentation, pre dissociation, production, decay. evidence for the existence of excited state and its types. Ions and electrons, radiolysis of gases. radiolysis of liquids, solids, and frozen liquids and gases, behaviour of ions in radiation chemistry: Ion recombination. dissociation and its types, charge transfer processes. ion-molecular reactions. electron addition. formation of free radicals, oxidation-reduction processes. Properties, reactions and detection of free radicals. Reactions in radiation chemistry: General energy transfer. characteristics and applications of gas, liquid and solid phase radiolysis. Instrumentation. purity of chemicals and methods, Recent applications of radiation chemistry. Radiation hazards and safe disposal of Radioactive wastes.

### **PHOTOCHEMISTRY**

Introduction. basic principles. and scope of photochemistry. Energy transfer in photochemical reactions. Fate of electron excitation, secondary reactions, quantum yield. reaction kinetics. Absorption and emission of radiation: Introduction to quantum efficiencies of emission processes, radiative and non-radiative processes. Beer-Lambert's law, spectroscopy and photochemistry. Emission processes, luminescence, kinetics and quantum efficiencies of radiative and non-radiative processes (fluorescence. phosphorescence, inter system crossing, internal conversion, quenching), and Stern-Volmer reactions. Photosensitized reactions, photo-stationary state. Applied photochemistry, Atmospheric photochemistry, photosynthesis, photochemistry of polymers, photo-medicines. Techniques in photochemistry, introduction, light source. incandescent filament lamps, discharge lamps, lasers, synchrotron reaction,

### **BOOKS RECOMMENDED**

1. Calvert JG and Pitts JN "Photochemistry" (1966) John Wiley, New York
2. Wayne and Richard P "Photochemistry" (1988) Macmillan
3. Hughes G "Radiation Chemistry" (1973) Oxford Series, UK
4. Spinks JWT and Woods RJ "An Introduction to Radiation Chemistry" (1976) Wiley Inter Sci. Pub, USA
5. O'Donnell JH and Sangster DF "*Principles of Radiation Chemistry*" (1970) Edward Arnold Pub, UK

6. Baco ZM and Alexander P "Fundamentals of Radiobiology" (1972) ELBS, UK
7. Suppan P "Principles of Photochemistry" (1973) The Chemical Sco, UK

### **CHM-626: CHEMICAL KINETICS**

Credit Hours: (3+0)

Correlation between physical property and concentration. Thermal decomposition of nitrogen pentoxide. Collision theory of reaction rates. Bimolecular and Unimolecular reaction theories. Transition state theory. Potential energy surfaces. Theory of absolute reaction rate. Derivation of the rate equation. Comparison of collision and absolute reaction theories.

Thermodynamic formulation of reaction rates. Calculation of entropy and enthalpy changes. Reversible reaction. Parallel reactions. Consecutive reactions.

Influence of ionic strength on the reaction rate. Reactions in solutions. Effect of dielectric constant of the medium on the rate of the reaction. Single sphere activated complex model. Double sphere activated complex model. Complex reactions. Chain reactions. Single chain carrier with second order breaking. One chain carrier with first order breaking. Two chain carrier with second order breaking. Experimental techniques for fast reactions.

Activation energy and catalysis. Mechanism of catalytic process. Kinetics of adsorption and desorption. Adsorption with dissolution. Mixed adsorption. Kinetics of surface catalyzed reactions. Unimolecular reactions. Bimolecular surface catalyzed reactions.

Reaction kinetics. Michealis- Menten, kinetics. Bell shape pH activity curve. Effect of pH on rate of enzyme catalysed reactions. Reversible reactions. Rate equations for Lineweaver- Bur equation. Woolf and Eisenthal and Cornish- Bowden methods. Non- competitive inhibition. Multi Substrate Reactions. Enzyme Inhibition.

### **BOOKS RECOMMENDED**

1. Frost AA and Pearson RG "Kinetic and Mechanism" 2<sup>nd</sup> Ed (1961) John Wiley and Sons Inc, New York
2. Laidler KJ "Chemical Kinetics" 2<sup>nd</sup> Ed (1965) Mc Graw Hill Book Company, New York
3. Laidler LJ "Reaction Kinetic VII, II Reaction in Solution" (1963) Pergamon Press, New York
4. Segal H "Enzyme Kinetics" (1975) John Wiley, New York
5. Schlutz AR "Enzyme Kinetics" (1964) Cambridge University Press England
6. Weston R and Schwavz HA "Chemical Kinetics" (1972) Prentice Hall Inc, New Jersey
7. Logan SR "Fundamentals of Chemical Kinetics" (1996) Longman Group Ltd, England
8. Smith WM "Kinetics and Dynamics of Elementary Gas Reactions" (1980) Butterworths and Co, London
9. Pilling MJ and Seaking PW "Reaction Kinetics" 2<sup>nd</sup> Ed (1996) Oxford University Press, New York
10. Konnars KA "Chemical Kinetics: The Study of Reaction Rates on Solution" (1990) VCH Publishers USA
11. Stenfeld JI, Francisco JS and Hase WL "Chemical Kinetics and Dynamics" 2<sup>nd</sup> Ed (1999) Prentice Int. Inc, New Jersey

### **CHM-636: RADIOCHEMISTRY**

Credit Hours: (3+0)

#### **INSIGHT INTO NUCLEAR DECAY PROCESS**

Atomic nucleus & modes of radioactive decay. Instability concepts, Radioisotopes. Units of radioactive decay process. Decay schemes Radioactive equilibrium.

#### **DETECTION METHODS**

Methods based on ion collection, Scintillation detectors, Semi conductor detectors. Discussions on specific applications of detection devices.

#### **STUDY OF LABELLED COMPOUNDS**

Preparation and dispersion of labelled compounds. Details of job oriented labelled compounds.

#### **STATISTICS OF RADIOACTIVE DECAY**

Decay rate and statistics. Practical consideration. Optimum counting rate. Background count. RADIATION

### **PROTECTION AND CONTROL**

Units of radiation exposure. Safety measures.

### **RADIOISOTOPES IN CHEMICAL APPLICATIONS**

Radiocarbon dating. Isotope dilution techniques Neutron activation analysis. Radiometric analysis  
Gravimetric methods. Radio immune assay. Applications of radioisotopes in pharmaceutical dispersions. Radio tracers in chemical applications. Study of self exchange reactions.

### **CHEMICAL EFFECT OF NUCLEAR DECAY**

An introduction to hot atom chemistry. Recoiling atoms. Chemical effects of nuclear transformations.

### **MOSBAUER SPECTROSCOPY**

Basic information, Experimental technique Parameters and chemical applications of Mosbauer spectroscopy.

### **BOOKS RECOMMENDED**

1. Geary WJ "Radio Chemical Methods" . (1986) John Wiley and Sons
2. Naqvi SII "Radiochemistry: Monograph" (1990) U.G.C. Islamabad
3. Vertes A "Basics of Nuclear Science" (2003) Kluwer Academic Publisher London

### **CHM- 646: CHEMICAL KINETICS PRACTICALS**

Credit Hours: (0+3)

Kinetic Study of the reaction between iodide and peroxodisulphats ions using spectrophotometric technique. Kinetic Study of the reaction between iodide and bromate ions. Kinetic Study of the reaction between bromide and bromate ions and evaluation of activation parameters.

Kinetics of fading of phenolphthalein in alkaline solution. Study of the effect of pH on the rate constant of the reaction between iodide and

persulphate ions. .Study of the salt effect on the rate constant of the reaction between similar charges of ions. Kinetics of autocatalytic reaction between permanganate and oxalate ions. .Determination of energy of activation of the reactions between similar charges of ions. Kinetics of the reaction between methylorange and peroxodisulphate ions in presence of bromide ion. Kinetics of the reaction between chloroacetate and thiosulphate ions.

#### **BOOKS RECOMMENDED**

1. James AM and Prichard FE "Practical Physical Chemistry" 3<sup>rd</sup> Ed (1974) Longman
2. Mowry S and Ogren PJ(1999) J Chemical Education 76 (7)
3. Birk JP and Watters DL "Kinetics of Halogenation of Acetone" (1992) J. Chemical Education 69 (7)
4. Shoemaker DP, Garland C W and Nibler JW "Experiments in Physical Chemistry" (1989) Mc Graw Hills, New York
5. Connors KA "Chemical Kinetics: The Study of Reaction Rates in Solution"
6. Wright MR "The introduction to Chemical Kinetics" (2004) John Wiley and Sons Ltd, UK
7. Pilling MJ and Seakins P W "Reaction Kinetics" (1996) Oxford University Press, UK

#### **CHM- 656 CONDUCTOMETRY LABS**

Credit Hours: (0+3)

#### **CONDUCTOMETRY**

Conductometric titration including acid-base neutralization of both strong and weak nature (and mixture of acids). Titration between salt of a weak acid vs. strong base. To study the displacement or replacement reaction. Precipitation and complexation reactions (determination of halides). Verification of Onsagar Equation by conductivity method for different electrolytes. Determination of dissociation constants of weak acids by conductivity method. Determination of molar conductivity of different electrolytes. Determination of basicity of a weak acid by conductivity method. Determination of solubility and solubility product of sparingly soluble salts. Determination of % of a mineral acid in the given vinegar solution. Determination of amount of ascorbic acid in a given tablet. Determination of acetyl salicylic acid in a given tablet. Determination of folic acid in a given tablet. Simultaneous determination of chromate and dichromate in a given sample. Determination of  $K_{sp}$ ,  $\Delta G$ ,  $\Delta S$ , and  $\Delta H$  for the dissolution of calcium hydroxide in water by conductivity method. Determination of

complexation reaction of copper with EDTA by conductivity.  
Determination of % of  $\text{Na}_2\text{CO}_3$  content of washing soda by conductivity determination of Ni with EDTA by conductivity method.

#### **BOOKS RECOMMENDED**

1. "Vogel's Textbook of Quantitative Inorganic Analysis" 6<sup>th</sup> Ed (1980) ELBS
2. Braun RD "Introduction to Chemical Analysis" (1983)
3. Heinemann S "Chemistry Experiments for Instrumental Methods" (1987)
4. Harris DC "Quantitative Chemical Analysis" 5<sup>th</sup> Ed (1998) W.H. Freeman & Co.
5. Euler WB et al. (2000) J Chemical Education 77(8) 1039
6. Kkalbus LH et al, (1991) J Chemical Education 68(8) 677

## List of Academic Staff

S#	Employee Name	Post
1.	Dr. Rehana Saeed	Professor
2.	Dr. Nasreen Fatima	Professor & (Chairperson)
3.	Dr. Firdous Imran Ali	Professor
4.	Dr. Itrat Anis	Professor
5.	Dr. Uzma Ashiq	Professor
6.	Dr. Sheikh Mohiuddin	Professor
7.	Dr. Erum Zahir	Professor
8.	Dr. Imran Ali Hashmi	Professor
9.	Dr. Rifat Ara Jamal	Associate Professor
10.	Dr. Shazia Nisar	Associate Professor
11.	Dr. Raheela Naz	Associate Professor
12.	Dr. Zahid Hussain	Associate Professor
13.	Dr. Syed Tariq Ali	Associate Professor
14.	Dr. Syed Kashif Ali	Associate Professor <b>(FSL)</b>
15.	Dr. Agha Arslan Wasim	Associate Professor
16.	Dr. Mohsin Ali	Associate Professor
17.	Dr. Saba Arslan Wasim	Associate Professor
18.	Dr. Tehseen Ahmed	Associate Professor
19.	Dr. Summyia Masood	Associate Professor
20.	Dr. Humaira Bano	Assistant Professor
21.	Dr. Naushaba Rafiq	Assistant Professor
22.	Dr. Syed Nawazish Ali	Assistant Professor
23.	Dr. Qurat-ul-Ain	Assistant Professor
24.	Dr. Hamida Sultan Muhammad	Assistant Professor <b>(FSL)</b>
25.	Dr. M. Asad Khan Tanoli	Assistant Professor

26.	Dr. Perveen Fazil	Assistant Professor
27.	Dr. Safi Asim Bin Asif	Assistant Professor
28.	Dr. Nizam Uddin	Assistant Professor
29.	Dr. Syed Muhammad Saad	Assistant Professor
30.	Dr. Maria Ashfaq Lodhi	Assistant Professor
31.	Dr. Noshab Qamar	Assistant Professor
32.	Dr. Sadaf Iqbal	Assistant Professor
33.	Dr. Nida Ali	Assistant Professor
34.	Dr. Fakhrun Nisa	Assistant Professor
35.	Dr. Muhammad Balal	Assistant Professor <b>(FSL)</b>
36.	Dr. Muhammad Saad	Assistant Professor

