B. Sc. Chemistry Syllabus

Four Year Undergraduate Programme (FYUGP)

DEPARTMENT OF CHEMISTRY

BHATTADEV UNIVERSITY, BAJALI

INTRODUCTION

The University Grants Commission (UGC) has initiated several measures to bring equity, efficiency and excellence in the Higher Education System of country. The important measures taken to enhance academic standards and quality in higher education include innovation and improvements in curriculum, teaching-learning process, examination and evaluation systems, besides governance and other matters. But due to the various diversities present in the system of higher education, there are multiple approaches followed by universities towards examination, evaluation and grading system. However, the academic reforms recommended by the UGC in the recent past have led to overall improvement in the higher education system. On the basis of the recommendation, apart from the flexibility and freedom in designing the examination, there is a need to devise a sensible system for awarding the grades based on the performance of students.

The National Education Policy (NEP) 2020 based Four-Year Undergraduate Programme (FYUGP), being adopted by Bhattadev University, is an 8-semester (4-year) programme of 160 credits with multiple exit and entry options at the successful completion of courses assigned at the end of each year.

• Students who opt to exit after completion of the first year and have secured 40 credits will be awarded a certificate if, in addition, they complete one vocational course of 4 credits during the summer vacation of the first year.

• Students who opt to exit after completion of the second year and have secured 80 credits will be awarded the diploma if, in addition, they complete one vocational course of 4 credits during the summer vacation of the second year.

• Students who opt to exit after completion of the third year and have secured 120 credits will be eligible for the Bachelor degree in the Major discipline without Honours.

• Students after completion of the fourth year and have secured 160 credits will be eligible for the Bachelor degree with Honours in the Major discipline.

• Students are allowed to re-enter the degree programme within three years and complete the degree programme within the stipulated maximum period of seven years.

Outline of Courses:

The broad categories of courses and minimum credits required for the 4-year Honours degrees as per the UGC document are as follows:

1. Major (Core) Course/Paper : 80 credits

2. Minor Course/Paper : 32 credits

3. Interdisciplinary Course/Paper (IDC) : 9 credits

4. Ability Enhancement Course/Paper (AEC) : 8 credits

5. Skill Enhancement Course/Paper (SEC) : 9 credits

6. Value Added Course/Paper (VAC) : 8 credits

7. Summer Internship : 2 credits

8. Research Project/ Dissertation : 12 credits (for Honours with Research degree)

The following points may be noted:

• In lieu of the Research Project, a student may study 3 courses each of 4 credits (i.e. total 12 credits), leading to an Honours degree (without Research).

• For the 4-year Honours degrees the Major subject/discipline requires 80 credits and the Minor subject/discipline requires 32 credits.

• For a Double Major, the minimum credit requirements are 48 (3-year degree) and 60 (4-year Honours degree) respectively in a subject/discipline other than the original Major.

• In the UGC framework, papers in Major and Minor disciplines are categorized into levels of 100, 200, 300 and 400.

Therefore, a course (paper) offered by a department, say with 4 credits and of level 200, may be taken both as a Major (Core) course by one student and as a Minor course by another student having a different Major discipline, possibly in different semesters.

Definition of Keywords:

In FYUGP the terminologies those are relevant to the B.Sc. curricula have been briefly described below.

Academic Year: Two consecutive (one odd + one even) semesters constitute one academic year.

Semester: Each semester will consist of 15 weeks of regular academic work. The odd semester may be scheduled from July to December and even semester from January to June under normal circumstance.

Programme: An educational programme leading to award of a Certificate, Diploma or Degree (B.Sc., B.A., etc.)

Discipline: This means a particular subject.

Course: Each programme is equipped with a number courses of various disciplines/subjects. The course of a particular discipline/subject refers to the content of the papers the students have to study in that

discipline/subject required in obtaining a degree. The courses should define learning objectives and learning outcomes. A course may be designed to comprise lectures /tutorials/laboratory work/ field work/outreach activities/project work /seminars /assignments/ presentations etc. or a combination of any of these.

Honours: A particular discipline/subject that a student opts as major subject. (e.g. Honours in Chemistry)

Core Course (CC): A discipline/subject specific compulsory basic course.

Skill Enhancement Course (SEC): A course designed by a department for enhancement of skill of the students in a particular discipline/subject.

Minor Course (M): A course in a discipline/subject corresponding to a subject other than the major subject.

Value Added Course (VAC): Value-based education to include management of biological resources and biodiversity for the development of humanistic, ethical, sustainable development and living, constitutional, and universal human values of truth, righteous conduct, peace, love, nonviolence, scientific temper, citizenship values, and life skills.

Ability Enhancement Compulsory Course (AECC): These are compulsory courses. For science programme there will be two of them. AECC-1 is Communicative English & AECC-2 is Environmental Science.

Vocational Course (VOC): A vocational course is focused on practical work, preparing students for a particular trade or skilled profession. These courses are best for students who have a good idea of their career path and want to gain the knowledge to get there.

Levels of Courses:

100 - 199 : Foundation or introductory courses.

200 - 299 : Intermediate level courses.

300 - 399 : Higher level courses.

400 - 499 : Advanced courses.

Credit: A unit by which the course work is measured. It determines the number of hours of instructions required per week. Theory/Tutorial classes: 1 credit = 1 hour/week and Practical classes: 1 credit = 2 hours/week

Credit Point: It is the product of grade point and number of credits for a course.

Letter Grade: It is an index of the performance of students in a said course.

Grade Point: It is a numerical weight allotted to each letter grade on a certain point scale.

The following table explains the above points

Letter Grade	Grade Point	Performane	Letter Grade	Grade Point	Performane
O	10	Outstanding	C+	5	Average
A+	9	Excellent	C	4	Pass
A	8	Very Good	F	0	Fail
B+	7	Good	I	0	Absent/Incomplete
B	6	Above Average			

Semester Grade Point Average (SGPA): It is a measure of performance of work done in a semester. It is ratio of total credit points secured by a student in various courses registered in a semester and the total course credits taken during that semester. It shall be expressed up to two decimal places. If C_i = credit point in the ith course/paper and G_i = grade point obtained by a student in the ith course/paper then the grade point average in the ith Semeter ie SGPA is given by $S_i = \frac{\sum C_i G_i}{\sum C_i}$.

Cumulative Grade Point Average (CGPA): It is a measure of overall cumulative performance of a student over all semesters. The CGPA is the ratio of total credit points secured by a student in various courses in all semesters and the sum of the total credits of all courses in all the semesters. It is expressed up to two decimal places. If S_i = Semester Grade point average in the ith Semeter and S = total number of semesters in the program, then the cumulative grade point average ie CGPA scored by the student is given by $C = \frac{\sum S_i}{\sum S}$.

Grade Sheet/Report: Based on the grades earned, a grade certificate shall be issued to all the registered students after every semester. The grade certificate will display the course details (code, title, number of credits, grade secured) along with SGPA of that semester and CGPA earned till that semester.

Lists of Courses:

CC :: Core Courses/Papers [For Degree with Chemistry (Major), 3 years UG program]

1. CHE1104C : Chemistry-I (Level: 100-199)

2. CHE2104C : Chemistry-II (Level: 100-199)

3. CHE3104C : Organic Chemistry-I (Level: 200-299)

4. CHE3204C : Physical Chemistry-I (Level: 200-299)

5. CHE4104C : Inorganic Chemistry-I(Level: 200-299)

6. CHE4204C : Organic Chemistry-II (Level: 200-299)

7. CHE4304C : Chemistry & Metallurgy [course based on Indian Knowledge System] (Level: 200-299)

8. CHE5104C : Inorganic Chemistry-II(Level: 300-399)

9. CHE5204C : Organic Chemistry-III(Level: 300-399)

10. CHE5304C : Physical Chemistry-II (Level: 300-399)

11. CHE5404C : Quantum Chemistry-I(Level: 300-399)

12. CHE6104C : Inorganic Chemistry-III(Level: 300-399)

13. CHE6204C : Organic Chemistry-IV(Level: 300-399)

14. CHE6304C : Physical Chemistry-III(Level: 300-399)

15. CHE6404C : Spectroscopy-I(Level: 300-399)

SEC :: Skill Enhancement Courses/Papers

1. CHE1103SE : Fuel Chemistry

2. CHE2103SE : Green Methods in Chemistry

3. CHE3103SE : Basic Analytical Chemistry

IDC :: Interdisciplinary Courses/Papers [Offered to the students of other discipline]

1. CHE1103ID : History of Chemistry

2. CHE2103ID : Environmental Chemistry

3. CHE3103ID : Chemistry in Humane Service

CC :: Core Courses/Papers [Additional Core Courses for degree with Chemistry (Honours) &Chemistry (Honours with Research)]

1. CHE7104C : Inorganic Chemistry-IV (Level: 400-499)

2. CHE7204C : Organic Chemistry-V (Level: 400-499)

3. CHE7304C : Physical Chemistry-IV (Level: 400-499)

4. CHE7404C : Research Methodology(Level: 400-499)

5. CHE8104C : Inorganic Chemistry-V (Level: 400-499)

6. CHE8204C : Organic Chemistry-VI (Level: 400-499)

7. CHE8304C : Physical Chemistry-V (Level: 400-499)

8. CHE8404C : Spectroscopy-II (Level: 400-499)

Research Project [For Chemistry (Honours with Research)]

1. CHE8512C : Research Project : In lieu of CHE8104C, CHE8204C andCHE8304C, a Research Project of Credit 12 has to be chosen for degree-Chemistry (Honours) with Research

Minor Courses/Papers (For students from other discipline)

1. CHE1104M : Chemistry-I (Level: 100-199)

2. CHE2104M : Chemistry-II (Level: 100-199)

3. CHE3104M : Chemistry-III(For Single Major) (Level: 200-299)

4. CHE3204M : Physical Chemistry-I(Additional Course to be chosen for Double Major along with CHE3104M)(Level: 200-299)

5. CHE4104M : Chemistry-IV(For Single Major) (Level: 200-299)

6. CHE4204M : Organic Chemistry-I (Additional Course to be chosen for Double Major)(Level: 200-299)

7. CHE5104M : Chemistry-V(For Single Major) (Level: 200-299)

8. CHE5204M : Inorganic Chemistry-I (Additional Course to be chosen for Double Major) (Level:200-299)

9. CHE5304M : Quantum Chemistry (Additional Course again to be chosen for Double Major along with CHE5104M & CHE5204M) (Level: 200-299)

10. CHE6104M : Chemistry-VI (For Single Major) (Level: 200-299)

11. CHE6204M : Organic Chemistry-II (Additional Course to be chosen for Double Major) (Level: 200-299)

12. CHE6304M : Spectroscopy (Additional Course again to be chosen for Double Major along with CHE6104M & CHE6204M) (Level: 200-299)

13. CHE7104M : Chemistry-VII(For Single Major) (Level: 300-399)

14. CHE7204M : Inorganic Chemistry-II (Additional course to be chosen for Double Major) (Level: 300-399)

15. CHE8104M : Chemistry-VIII(For Single Major) (Level: 300-399)

16. CHE8204M: Physical Chemistry-II (Additional course to be chosen for Double Major) (Level: 300-399)

Course Structure for BSc Chemistry (H) under FYUGP

Semester	CC-1 Credit-4	CC-2 Credit-4	AEC Credit-2	SEC Credit-3	IDC Credit-3	VAC Credit-4	Internship Credit-2
SEM-I	Chemistry-I	To be chosen from other department	A common course of	Basic analytical chemistry	To be chosen from other department	A comm on course	N/A
SEM-II	Chemistry-II	To be chosen from other department	A common course of	Green methods in chemistry	To be chosen from other department	A comm on course	N/A

To EXIT with a Certificate after one year, a mandatory VOC of credit 4 has to be chosen or proceed to the 2nd year.

Semester	Major/CC Credit-4	Minor Credit-4	AEC Credit-2	SEC Credit-3	IDC Credit-3	VAC Credit-4	Internship Credit-2
SEM-III	Organic Chemistry-I Physical Chemistry-I	To be chosen from other department	A common course	Fuel chemistry	To be chosen from other department	N/A	N/A
SEM-IV	Inorganic Chemistry-I Organic Chemistry-II Chemistry and Metallurgy (IKS based)	To be chosen from other department	A common course	N/A	N/A	N/A	Has to be engaged in an summer internship

To EXIT with a Diploma after one year, a mandatory VOC of credit 4 has to be chosen or Proceed to the 3rd year.

Semester	Major/CC Credit-4	Minor Credit-4	AEC Credit-2	SEC Credit-3	IDC Credit-3	VAC Credit-4	Internship Credit-2
SEM-V	Inorganic Chemistry-II Organic Chemistry-III Physical Chemistry-II Quantum Chemistry-I	To be chosen from other department	N/A	N/A	N/A	N/A	N/A
SEM-VI	Inorganic Chemistry-III Organic Chemistry-IV Physical Chemistry-III Spectroscopy-I	To be chosen from other department	N/A	N/A	N/A	N/A	N/A

EXIT Option with a Bachelor degree after three years or Proceed to the 4th year.

Semester	Major/CC Credit-4	Minor Credit-4	AEC Credit-2	SEC Credit-3	IDC Credit-3	VAC Credit-2	Internship Credit-2
SEM-VII	Inorganic Chemistry-IV Organic Chemistry-V Physical Chemistry-IV Research Methodology	To be chosen from other department	N/A	N/A	N/A	N/A	N/A
SEM-VIII	Inorganic Chemistry-V Organic Chemistry-VI Physical Chemistry-V Spectroscopy-II	To be chosen from other department	N/A	N/A	N/A	N/A	N/A

CC: CORE COURSES/PAPER

CHE1104C: Chemistry-I

Total lectures: 45(L + T) & 30 (P) Credits: 4 (Theory: 03, Lab: 01)

Course Objective: *This course may be divided into three broad areas of chemistry- physical, organic and inorganic chemistry. In this course students will be taught basics of organic chemistry, atomic structure, gaseous and liquid state.*

Learning Outcome: *After completion of this course the students will learn the atomic structure through the basic concepts of quantum mechanics. They will learn about the states of matter, especially gaseous and liquid states. In organic part, the students are expected to learn basic ideas used in organic chemistry.*

Gaseous State: (**10h**)

Kinetic molecular model of a gas: postulates and derivation of the kinetic gas equation; collision frequency; collision diameter; mean free path and viscosity of gases, including their temperature and pressure dependence, relation between mean free path and coefficient of viscosity, calculation of σ from η; variation of viscosity with temperature and pressure.

Maxwell distribution and its use in evaluating molecular velocities (average, root mean square and most probable) and average kinetic energy.

Behaviour of real gases: Deviations from ideal gas behaviour, compressibility factor, Z, and its variation with pressure for different gases. Causes of deviation from ideal behaviour. Vander Waals equation of state, its derivation and application in explaining real gas behaviour, Boyle temperature. critical state, relation between critical constants and van der Waals constants, law of corresponding states.

Liquid State: (**5h)**

Physical properties of liquids; vapour pressure, surface tension and coefficient of viscosity, and their determination. Effect of addition of various solutes on surface tension and viscosity. Temperature variation of viscosity of liquids and comparison with that of gases.

Basics of Organic Chemistry: (15h)

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

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

Homolytic and Heterolytic fission with suitable examples. Curly arrow rules, formal charges;Electrophiles and Nucleophiles; Nucleophlicity and basicity; Types, shape and their relative stability of Carbocations, Carbanions, Free radicals and Carbenes.

Introduction to types of organic reactions and their mechanism: Addition, Elimination and Substitution reactions.

Aromaticity: Hückel's rule, aromatic character of arenes, cyclic carbocations/carbanions and heterocyclic compounds with suitable examples.

Atomic Structure: (15h)

Bohr's theory, its limitations and atomic spectrum of hydrogen atom. Wave mechanics: de Broglie equation, Heisenberg's Uncertainty Principle and its significance, Schrödinger's wave equation, significance of ψ and ψ^2. Quantum numbers and their significance. Normalized and orthogonal wave functions. Sign of wave functions. Radial and angular wave functions for hydrogen atom. Radial and angular distribution curves. Shapes of *s, p, d* and *f* orbitals. Contour boundary and probability diagrams. Pauli's Exclusion Principle, Hund's rule of maximum multiplicity, Aufbau's principle and its limitations, Variation of orbital energy with atomic number.

Recommended Books:

1.Lee, J. D. *Concise Inorganic Chemistry*, 5th Ed., Oxford University Press, 2008.
2. Douglas, B.E. and Mc Daniel, D.H., *Concepts and Models of Inorganic Chemistry*, 3rd Ed. Wiley India, 2006.
3. Morrison, R. N. & Boyd, R. N. *Organic Chemistry*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
4. Finar, I. L. *Organic Chemistry (Volume 1),* Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
5. Peter, A. & Paula, J. de. *Physical Chemistry 9th Ed*., Oxford University Press (2011).
6. Castellan, G. W. *Physical Chemistry* 4th Ed., Narosa (2004).
7. Advanced Organic Chemistry; Reactions, Mechanisms and Structure; Jerry March

LAB: (30 h)

(i) Detection N, S, halogens in organic compounds.
(ii) Detection of Functional groups present in organic samples.
(iii) Titrimetric Analysis
    (a) Calibration and use of common laboratory apparatus
    (b) Preparation of solutions of different Molarity/Normality of titrants

Recommended Books:

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

3. Ahluwalia, V.K. & Aggarwal, R. *Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis*, University Press (2000).
4. Khosla, B. D.; Garg, V. C. & Gulati, A., *Senior Practical Physical Chemistry*, R. Chand & Co.: New Delhi (2011).

CHE2104C: Chemistry-II

Total lectures: 45(L + T) & 30 (P) Credits: 4 (Theory: 03, Lab: 01)

Course Objective: *This course may be divided into three broad areas of chemistry- physical, organic and inorganic chemistry. In this course students will be taught solid state, ionic equilibria, stereochemistry and periodicity of elements.*

Learning Outcome: *After completion of this course the students will learn the fundamental concepts of solid state and ionic equilibria along with conductance. They will understand the periodic properties of elements. In organic part, the students are expected to learn basic ideas stereochemistry.*

Solid State: (4h)

Nature of the solid state, law of constancy of interfacial angles, law of rational indices, Miller indices; X-ray diffraction, Bragg's law, a simple account of rotating crystal method and powder pattern method. Analysis of powder diffraction patterns of NaCl, CsCl and KCl. Defects in crystals. Liquid crystals (Introductory idea)

Ionic equilibria and Conductance: (11h)

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

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

Solubility and solubility product of sparingly soluble salts – applications of solubility product principle. Qualitative treatment of acid – base titration curves (calculation of pH at various stages). Theory of acid–base indicators; selection of indicators and their limitations.

Multistage equilibria in polyelectrolyte systems; hydrolysis and hydrolysis constants.

Arrhenius theory of electrolytic dissociation. Conductivity, equivalent and molar conductivity and their variation with dilution for weak and strong electrolytes. Molar conductivity at infinite dilution. Kohlrausch law of independent migration of ions. Debye-Hückel-Onsager equation, Wien effect, Debye-Falkenhagen effect, Walden's rules.

Stereochemistry: **(15 h)**

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

Optical Isomerism: Optical Activity, Specific Rotation, Chirality/Asymmetry, Enantiomers

Molecules with two or more chiral-centres, Distereoisomers, meso structures, Racemic mixture and resolution. Relative and absolute configuration: D/L and R/S designations. Atropisomerism and their R/S designation.

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

Periodicity of Elements: **(15 h)**

Long form of periodic table. s, p, d, f block elements. Detailed discussion of the following properties of the elements, with reference to s & p-block:
(a) Effective nuclear charge, shielding or screening effect, Slater rules, variation of effective nuclear charge in periodic table.
(b) Atomic radii (van der Waals)
(c) Ionic and crystal radii.
(d) Covalent radii (octahedral and tetrahedral)
(e) Ionization enthalpy, Successive ionization enthalpies and factors affecting ionization energy. Applications of ionization enthalpy.
(f) Electron gain enthalpy, trends of electron gain enthalpy.
(g) Electronegativity, Pauling's/Mulliken's/Allred Rachow's/ and Mulliken-Jaffé's electronegativity scales. Variation of electronegativity with bond order, partial charge, hybridization, group electronegativity. Sanderson's electron density ratio.

Recommended Books

1.Lee, J. D. *Concise Inorganic Chemistry*, 5th Ed., Oxford University Press, 2008.
2. Douglas, B.E. and Mc Daniel, D.H., *Concepts and Models of Inorganic Chemistry*, 3rd Ed. Wiley India, 2006.
3. Morrison, R. N. & Boyd, R. N. *Organic Chemistry*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
4. Finar, I. L. *Organic Chemistry* (Volume 1), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
5. Peter, A. & Paula, J. de. *Physical Chemistry* 9th Ed., Oxford University Press (2011).
6. Castellan, G. W. *Physical Chemistry* 4th Ed., Narosa (2004).

LAB: **(30 h)**

Acid-Base Titrations
(i) Estimation of carbonate and hydroxide present together in mixture.
(ii) Estimation of carbonate and bicarbonate present together in a mixture.
(iii) Estimation of free alkali present in different soaps/detergents
Oxidation-Reduction Titrimetry
(i) Estimation of Fe(II) and oxalic acid using standardized $KMnO_4$solution.

(ii) Estimation of oxalic acid and sodium oxalate in a given mixture.
(ii) Estimation of Fe(II) with $K_2Cr_2O_7$using internal (diphenylamine, anthranilic acid) and external indicator

Recommended Books:

1. Mann, F.G. & Saunders, B.C. *Practical Organic Chemistry*, Pearson Education (2009)
2. Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. *Practical Organic Chemistry*, 5th Ed., Pearson (2012)
3. Ahluwalia, V.K. & Aggarwal, R. *Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis*, University Press (2000).
4. Khosla, B. D.; Garg, V. C. & Gulati, A., *Senior Practical Physical Chemistry*, R. Chand & Co.: New Delhi (2011).
5. Mendham, J. et al.: *Vogel's Text Book of Quantitative Chemical Analysis*; 6th Ed. Pearson Education, 2009.

CHE3104C: Organic Chemistry-I

Total lectures: 45(L + T) & 30 (P) Credits: 4 (Theory: 03, Lab: 01)

Course Objectives: *This course is intended to apprise students about different classes of organic compounds, including halogenated hydrocarbons, alcohols, phenols, epoxides, carbonyl compounds and carboxylic and sulfonic acids. Students are expected to learn and differentiate between various organic functional groups; explain, analyze and design transformations between different functional groups.*
Learning Outcome: *Students will be able to describe and classify organic compounds in terms of their functional groups and reactivity.*

Chemistry of Aliphatic Hydrocarbons: (10 h)

Carbon-Carbon sigma bonds:

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

Carbon-Carbon pi bonds:

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

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

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

Electrophilic Aromatic Substitution: (5 h)

Halogenation, nitration, sulphonation and Friedel-Craft's alkylation/acylation with their mechanism. Directing effects of the groups.

Alkyl and Aryl Halides: (10 h)

Alkyl halides: Methods of preparation, nucleophilic substitution reactions – SN1, SN2 and SNi mechanisms with stereochemical aspects and effect of solvent etc.; nucleophilic substitution vs. elimination.

Aryl halides: Preparation, including preparation from diazonium salts. nucleophilic aromatic substitution; SNAr, Benzyne mechanism. Relative reactivity of alkyl, allyl/benzyl, vinyl and aryl halides towards nucleophilic substitution reactions.

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

Alcohols, Phenols, Ethers and Epoxides: (10 h)

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

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

Ethers and Epoxides: Preparation and reactions with acids. Reactions of epoxides with alcohols, ammonia derivatives and $LiAlH_4$

Carbonyl Compounds: (10h)

Preparation, properties, structure and reactivity;

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

Addition reactions of unsaturated carbonyl compounds: Michael addition.

Active methylene compounds: Keto-enol tautomerism. Preparation and synthetic applications of diethyl malonate and ethyl acetoacetate.

Recommended Books:

1. Morrison, R. N. & Boyd, R. N. *Organic Chemistry*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
2. Finar, I. L. *Organic Chemistry* (Volume 1), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
3. Eliel, E. L. & Wilen, S. H. *Stereochemistry of Organic Compounds*, Wiley: London, 1994.
4. Nasipuri, D. *Stereochemistry of Organic Compounds*, Wiley Eastern Limited.
5. Kalsi, P. S. *Stereochemistry Conformation and Mechanism*, New Age International, 2005.
6. Subrata Sen Gupta, *Basic Stereochemistry of Organic Molecules*, Oxford Higher Education.
7. Dhillon, R. S.; Singh, I. P. & Baskar, C. *Stereochemistry*, Narosa.
8. Loudon, G. M. *Organic Chemistry*, Oxford.
9. Sykes, P. *A guidebook to Mechanism in Organic Chemistry*, Pearson Education, 2003.
10. Clayden, J., Greeves, N. & Warren, S. *Organic Chemistry*, Second edition, Oxford University Press, 2012.

LAB: (30 h)

1. Checking the calibration of the thermometer
2. Purification of organic compounds by crystallization using the following solvents:
    a. Water
    b. Alcohol
    c. Alcohol-Water
3. Determination of the melting points of above compounds and unknown organic Compounds.
4. Effect of impurities on the melting point – mixed melting point of two unknown organic Compounds.
5. Determination of boiling point of liquid compounds. (boiling point lower than and more than 100 °C by distillation and use of thiele tube method)
6. Chromatography
    a. Separation of a mixture of two amino acids by ascending and horizontal paper chromatography
    b. Separation of a mixture of two sugars by ascending paper chromatography
    c. Separation of a mixture of o-and p-nitrophenol or o-and p-aminophenol by thin layer chromatography (TLC)

Recommended Books:

1. Mann, F.G. & Saunders, B.C. *Practical Organic Chemistry*, Pearson Education (2009).
2. Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. *Practical Organic Chemistry, 5th Ed.,* Pearson (2012)
3. Vogel, A. I. *Elementary Practical Organic Chemistry*, Part 2: *Qualitative Organic Analysis*, CBS Publishers and Distributors.
4. Bhattacharyya, R. C, *A Manual of Practical Chemistry.*
5. Dutta, S, *B. Sc. Honours Practical Chemistry*, Bharati Book Stall.

CHE3204C: Physical Chemistry-I

Total lectures: 45(L+T) & 30 (P) Credits: 4 (Theory: 03, Lab: 01)

Course Objective: *In this course the chemical thermodynamics, chemical equilibrium, solutions and colligative properties will be taught to the students. Another unit of this course is systems of variable compositions.*

Learning Outcome: *In this course the students are expected to learn laws of thermodynamics, thermochemistry, thermodynamic functions, relations between thermodynamic properties, Gibbs Helmholtz equation, Maxwell relations etc. Moreover, the students are expected to learn partial molar quantities, chemical equilibrium, solutions and colligative properties. After completion of this course, the students will be able to understand the chemical systems from thermodynamic point of view.*

Chemical Thermodynamics-I: (12h)

Intensive and extensive variables; state and path functions; isolated, closed and open systems; zeroth law of thermodynamics.
First law: Concept of heat, *q*, work, *w*, internal energy, *U*, and statement of first law; enthalpy, *H*, relation between heat capacities, calculations of *q*, *w*, *U* and *H* for reversible, irreversible and free expansion of gases (ideal and van der Waals) under isothermal and adiabatic conditions. Law of equipartition of energy, degrees of freedom and molecular basis of heat capacities.
Thermochemistry: Heats of reactions: standard states; enthalpy of formation of molecules and ions and enthalpy of combustion and its applications; calculation of bond energy, bond dissociation energy and resonance energy from thermochemical data, effect of temperature (Kirchhoff's equations) and pressure on enthalpy of reactions. Adiabatic flame temperature, explosion temperature.

Chemical Thermodynamics-II: (18h)

Second Law: Concept of entropy; thermodynamic scale of temperature, statement of the second law of thermodynamics; molecular and statistical interpretation of entropy. Calculation of entropy change for reversible and irreversible processes.

Third Law: Statement of third law, concept of residual entropy, calculation of absolute entropy of molecules.

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

*Systems of Variable Composition***:** Partial molar quantities, dependence of thermodynamic parameters on composition; Gibbs-Duhem equation, chemical potential of ideal mixtures, change in thermodynamic functions in mixing of ideal gases.

Chemical Equilibrium: (8h)

Criteria of thermodynamic equilibrium, degree of advancement of reaction, chemical equilibria in ideal gases, concept of fugacity. Thermodynamic derivation of relation between Gibbs free energy of reaction and reaction quotient. Coupling of exoergic and endoergic reactions. Equilibrium constants and their quantitative dependence on temperature, pressure and concentration. Free energy of mixing and spontaneity; thermodynamic derivation of relations between the various equilibrium constants K_p, K_c and K_x. Le Chatelier principle (quantitative treatment); equilibrium between ideal gases and a pure condensed phase.

Solution and Colligative Properties: (7h)

Dilute solutions; lowering of vapour pressure, Raoult's and Henry's Laws and their applications. Excess thermodynamic functions. Thermodynamic derivation using chemical potential to derive relations between the four colligative properties [(i) relative lowering of vapour pressure, (ii) elevation of boiling point, (iii) Depression of freezing point, (iv) osmotic pressure] and amount of solute. Applications in calculating molar masses of normal, dissociated and associated solutes in solution.

Recommended Books:

1. Peter, A. & Paula, J. de. *Physical Chemistry 9th Ed.,* Oxford University Press (2011).
2. Castellan, G. W. *Physical Chemistry 4th Ed.,* Narosa (2004).
3. Engel, T. & Reid, P. *Physical Chemistry 3rd Ed.,* Prentice-Hall (2012).
4. McQuarrie, D. A. & Simon, J. D. *Molecular Thermodynamics* Viva Books Pvt. Ltd.: New Delhi (2004).
5. Assael, M. J.; Goodwin, A. R. H.; Stamatoudis, M.; Wakeham, W. A. & Will, S. *Commonly Asked Questions in Thermodynamics.* CRC Press: NY (2011).
6. Levine, I .N. *Physical Chemistry* 6th Ed., Tata Mc Graw Hill (2010).
7. Metz, C.R. *2000 solved problems in chemistry,* Schaum Series (2006)
8. Puri, B. R.; Sharma, L. R.; Pathania, M. S. Principles of Physical Chemistry, Vishal Publishing Co.; 47th Ed. (2017)
9. Kapoor, K. L. A Textbook of Physical Chemistry (Volume 2) McGraw Hill Education; Sixth edition (2019)

LAB: **(30h)**

Thermochemistry

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

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

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

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

(e) Determination of basicity/proticity of a polyprotic acid by the thermochemical method in terms of the changes of temperatures observed in the graph of temperature versus time for different additions of a base. Also calculate the enthalpy of neutralization of the first step.

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

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

Recommended Books:

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

CHE4104C: Inorganic Chemistry-I

Total lectures: 45(L+T) & 30 (P) Credits: 4 (Theory: 03, Lab: 01)

Course Objective: *This course introduces structure and bonding in/of these are to be dealt with basic quantum chemistry treatment. Reactivity of chemical species based on their electron transfer affinity is introduced. Periodic behavior of s and p block elements related to their electronic structure and their reactivity is included to acquaint students with the principles governing their reactivity. This course further intend to apprise students about the variety of compounds of the main group elements including oxides, hydrides, nitrides, interhalogens.*

Learning Outcome: *On successful completion, students would have clear understanding of the concepts related to atomic and molecular structure, chemical bonding. Students will be able to identify the variety of s and p block compounds and comprehend their preparation, structure, bonding, properties and uses. Experiments in this course will boost their quantitative estimation skills and introduce the students to preparative methods in inorganic chemistry.*

Chemical Bonding: (20 h)

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

(ii) Covalent bond: Lewis structure, Valence Bond theory (Heitler-London approach). Energetics of hybridization, equivalent and non-equivalent hybrid orbitals. Bent's rule, Resonance and resonance energy, Molecular orbital theory. Molecular orbital diagrams of diatomic and simple polyatomic molecules N_2, O_2, C_2, B_2, F_2, CO, NO, and their ions; HCl, BeF_2, CO_2, (idea of s-p mixing and orbital interaction to be given). Formal charge, Valence shell electron pair repulsion theory (VSEPR), shapes of simple molecules and ions containing lone pairs and bond pairs of electrons, multiple bonding (σ and π bond approach) and bond lengths. Covalent character in ionic compounds, polarizing power and polarizability. Fajan's rules and consequences of polarization. Ionic character in covalent compounds: Bond moment and dipole moment. Percentage ionic character from dipole moment and electronegativity difference.

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

(iv) Weak Chemical Forces: van der Waals forces, ion-dipole forces, dipole-dipole interactions, induced dipole interactions, Instantaneous dipole-induced dipole interactions. Repulsive forces, Hydrogen bonding

(theories of hydrogen bonding, valence bond treatment) Effects of chemical force, melting and boiling points, solubility energetics of dissolution process.

Chemistry of *s* and *p* Block Elements: **(20 h)**

Inert pair effect, Relative stability of different oxidation states, diagonal relationship and anomalous behaviour of first member of each group. Allotropy and catenation. Complex formation tendency of s and p block elements. Hydrides and their classification ionic, covalent and interstitial. Basic beryllium acetate. Study of the following compounds with emphasis on structure, bonding, preparation, properties and uses. Boric acid and borates, boron nitrogen compounds, boranes, carboranes and graphitic compounds, silanes, oxides and oxoacids of nitrogen, sulphur, phosphorus and chlorine.

Interhalogen compounds, polyhalide ions, pseudohalogens and basic properties of halogens.

Noble Gases: **(5 h)**

Occurrence and uses, rationalization of inertness of noble gases, clathrates, preparation and properties of XeF_2, XeF_4 and XeF_6. Nature of bonding in noble gas compounds (VBT and MOT treatment for XeF_2). Molecular shape of noble gas compounds (VSEPR theory).

Recommended Books:

1. Lee, J. D., *Concise Inorganic Chemistry*, 5th Ed., Oxford University Press, 2008.

2. Douglas, B.E. and Mc Daniel, D.H., *Concepts and Models of Inorganic Chemistry*, 3rdEd. Wiley India, 2006.

3. Greenwood, N.N. & Earnshaw, A., *Chemistry of the Elements*, 2nd Ed., Elsevier India, 2010.

4. Cotton, F.A., Wilkinson, G. and Gaus, P. L., *Basic Inorganic Chemistry*, 3rd Ed., Wiley, 2007.

5. Cotton, F.A. & Wilkinson, G, *Advanced Inorganic Chemistry*. 6th Ed., Wiley-VCH, 2007.

6. Miessler, G. L. & Tarr, D. A., *Inorganic Chemistry* 4th Ed., Pearson, 2010.

LAB: **(30 h)**

(A) Iodo / Iodimetric Titrations:

(i) Estimation of Cu(II) and $K_2Cr_2O_7$ using sodium thiosulphate solution (Iodimetrically).

(ii) Estimation of (i) arsenite and (ii) antimony in tartar-emetic iodimetrically

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

(B) Inorganic preparations

(i) Cuprous Chloride, CuCl

(ii) Preparation of manganese(III) phosphate, $MnPO_4.H_2O$

(iii) Preparation of aluminium potassium sulphate $KAl(SO_4)_2.12H_2O$ (Potash alum) or Chrome alum.

Recommended Books:

1. Mendham, J. et al.: *Vogel's Text Book of Quantitative Chemical Analysis* ; 6th Ed. Pearson Education, 2009.

2. Marr, G. and Rockett, R.W. *Practical Inorganic Chemistry*, Van NostrandReinhold. 1972.

CHE4204C: Organic Chemistry-II

Total lectures: 45(L+T) & 30 (P) Credits: 4 (Theory: 03, Lab: 01)

Course Objective*: The course intrudes students to different classes of N-based compounds, including alkaloids and terpenoids and their potential application. Students are expected to learn about different classes of N-based compounds; their structures, synthesis and reactivity.*
Learning Outcome: *Students shall demonstrate the ability to identify and classify different types of N-based derivatives, alkaloids and heterocyclic compounds/explain their structure mechanism and reactivity/critically examine their synthesis and reactions mechanism.*

Carboxylic Acids and their Derivatives: (10 h)

Preparation, physical properties and reactions of monocarboxylic acids: Typical reactions of dicarboxylic acids, hydroxy acids and unsaturated acids: succinic/phthalic, lactic, malic, tartaric, citric, maleic and fumaric acids.

Preparation and reactions of acid chlorides, anhydrides, esters and amides; Comparative study of nucleophilic substitution at acyl group -Mechanism of acidic and alkaline hydrolysis of esters, Claisen condensation, Dieckmann and Reformatsky reactions, Hofmann bromamide degradation and Curtius rearrangement.

Sulphur and Nitrogen Containing Compounds: (15h)

Preparation and reactions of thiols, thioethers and sulphonic acids.

Preparation and important reactions of nitro and compounds, nitriles and isonitriles.

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

Diazonium Salts: Preparation and their synthetic applications.

Heterocyclic Compounds: (10h)

Classification and nomenclature, Structure, aromaticity in 5-numbered and 6-membered rings containing one heteroatom;

Synthesis, reactions and mechanism of substitution reactions of: Furan, Pyrrole (Paal-Knorr synthesis, Knorr pyrrole synthesis, Hantzsch synthesis), Thiophene, Pyridine (Hantzsch synthesis), Pyrimidine. Indole: Fischer indole synthesis and Madelung synthesis).

Polynuclear Aromatic Hydrocarbons: (10h)

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

Recommended Books:

1. Morrison, R. T. & Boyd, R. N. *Organic Chemistry*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
2. Finar, I. L. *Organic Chemistry* (*Volume 1*), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
3. Graham Solomons, T.W. *Organic Chemistry,* John Wiley & Sons, Inc.
4. Clayden, J., Greeves, N. & Warren, S. *Organic Chemistry,* Second edition, Oxford University Press, 2012.
5. Keeler, J., Wothers, P. *Chemical Structure and Reactivity – An Integrated approach*, Oxford University Press.
6. Smith, J. G. *Organic Chemistry*, Tata McGraw-Hill Publishing Company Limited.
7. Carey, F. A.; Sundberg, R. J. *Advanced Organic Chemistry: Reactions and Synthesis (Part B)*, Springers.

LAB: (30 h)

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

2. Organic preparations:
i. Acetylation of one of the following compounds: amines (aniline, *o*-, *m*-, *p*-toluidines*o*-, *m*-, *p*-anisidine) and phenols (β-naphthol, vanillin, salicylic acid) by any one method:
   a. Using conventional method.
   b. Using green approach
ii. Benzolyation of one of the following amines (aniline, *o*-, *m*-, *p*- toluidines and *o*-, *m*-, *p*-anisidine) and one of the following phenols (β-naphthol, resorcinol, pcresol) by Schotten-Baumann reaction.
iii. Oxidation of ethanol/ isopropanol (Iodoform reaction).
iv. Bromination of any one of the following:
   a. Acetanilide by conventional methods
   b. Acetanilide using green approach (Bromate-bromide method)

v. Nitration of any one of the following:

a. Acetanilide/nitrobenzene by conventional method

b. Salicylic acid by green approach (using ceric ammonium nitrate). vi. Selective reduction of *meta* dinitrobenzene to *m*-nitroaniline.

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

viii. Hydrolysis of amides and esters.

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

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

xi. Aldol condensation using either conventional or green method.

xii. Benzil-Benzilic acid rearrangement.

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

Recommended Books:

1. Mann, F.G. & Saunders, B.C. *Practical Organic Chemistry*, Pearson Education (2009)

2. Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. *Practical Organic Chemistry, 5th Ed.,* Pearson (2012)

3. Ahluwalia, V.K. & Aggarwal, R. *Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis,* University Press (2000).

4. Ahluwalia, V.K. & Dhingra, S. *Comprehensive Practical Organic Chemistry: Qualitative Analysis,* University Press (2000).

5. Vogel, A. I. *Elementary Practical Organic Chemistry,* Part 1: *Small scale Preparations,* CBS Publishers and Distributors.

CHE4304C: Chemistry and Metallurgy (based on Indian Knowledge System)

Total lectures: 60 (L+T) Credits: 4 (Theory: 04, Lab: 00)

Course Objective: *The course is intended to provide students with a foundational guide to the ancient chemistry of India and introduce them to the main themes and debates relating to that history and modern chemistry.*

Learning Outcome: *On completion of this course the students will include knowledge from ancient India and its contributions to modern India and its successes.*

Theoretical Framework for the Practice of Science in Ancient India: (10 h)

Chemistry in practice as gleaned from the medical schools of ancient India, Qualities of compounds; formation of molecular properties in chemical compounds, Chemistry of colors, measures of weight and capacity, size of the minimum visible.

Metallurgical Heritage: (10 h)

Arthaśāstra as the earliest text describing gold, silver, and other metals; Processing of gold, silver, copper, iron, tin, mercury, and lead as mentioned in the Indian texts in the ancient and Medieval Period, Zinc distillation as mentioned in Rasārṇava and Rasaratnasamukāyā.

Material Chemistry, Textile Chemistry & Pyro Technology: (20 h)

Copper/Bronze/Zinc: Important Mines (Zawar, Khetri mines); Iron and Wootz Steel Technology; Textile and Dyeing- Indian Specialities (Kutchi Embroidery, Cotton Textile etc.); Ceramic Technology, Stone (Lapidary), Shell, Ivory, Faience & Glass Technology, Zeolites, Clay, Inorganic polymer.

Concepts of Acids and Bases: (20 h)

Brönsted-Lowry concept of acid-base reactions, solvated proton, relative strength of acids, types of acid-base reactions, levelling solvents, Lewis acid-base concept, Classification of Lewis acids, Hard and Soft Acids and Bases (HSAB), Application of HSAB principle, non-aqueous solvent.

Concepts of acid and bases in Indian chemistry from organic fruit, vegetable-based; Acids, plant-ash-based bases to mineral acids of the medieval period.

Recommended Books:

1. Seal, B. N. *The Positive Sciences of the Ancient Hindus*; 4th Edition (2016).

2. Bose, D. M.; Sen, S. N.; Subbarayappa, B. V.; *A Concise History of Science in India*, INSA (2009).

3. Rahman, A.; Alvi, M. A.; Khan Ghori, S. A.; Samba Murthy, K. V.; *Science and Technology in Medieval India - A Bibliography of Source Materials in Sanskrit, Arabic and Persian* (1982).

4. Tripathi, V. Ed. *Archaeometallurgy in India*, (Cambridge University Press, 1998).

5. Huheey, J. E., Keiter, E. A., Keiter, R. L., Medhi, O. K., *Inorganic Chemistry: Principles of Structure and Reactivity*, 4th Ed., Pearson Education India, 2006.

CHE5104C: Inorganic Chemistry-II

Total lectures: 45(L+T) & 30 (P) Credits: 4 (Theory: 03, Lab: 01)

Course Objective: *This course introduces students to coordination chemistry. Various aspects like nomenclature, structure, bonding, variety and reactivity of the coordination compounds are included for the students to appreciate. Bioinorganic chemistry is included in this course to acquaint students on the useful and harmful aspects of metals in biological systems. Through the accompanying lab course, experiments related to gravimetric analysis, synthesis of coordination compounds and separation of metal ions using chromatography is included. This will broaden the experimental skills of the students where students will learn about various aspects of experiment design depending upon the requirements like synthesis, estimation or separation.*

Learning Outcome: *On successful completion, students will be able name coordination compounds according to IUPAC, explain bonding in this class of compounds, understand their various properties in terms of CFSE and predict reactivity. Students will be able to appreciate the general trends in the properties of transition elements in the periodic table and identify differences among the rows. Through the experiments students not only will be able to prepare, estimate or separate metal complexes/compounds but also will be able to design experiments independently which they should be able to apply if and when required.*

Coordination Chemistry: (20 h)

Coordination compounds, types of ligands, Werner's theory, IUPAC nomenclature and isomerism in coordination compounds. Stereochemistry of complexes with 4 and 6 coordination numbers. Valence bond theory (inner and outer orbital complexes), electroneutrality principle and back bonding. Crystal field theory, measurement of 10 Dq (Δ_o), CFSE in weak and strong fields, pairing energies, factors affecting the magnitude of 10 Dq (Δ_o,Δ_t).Octahedral vs. tetrahedral coordination, tetragonal distortions from octahedral geometry Jahn-Teller theorem, square planar geometry. Qualitative aspects of ligand field and MO Theory. Chelate effect, polynuclear complexes.

Transition Elements: (12 h)

General group trends with special reference to electronic configuration, colour, variable valency, magnetic and catalytic properties, ability to form complexes. Stability of various oxidation states and e.m.f. (Latimer & Frost diagrams). Difference between the first, second and third transition series.
Chemistry of Ti, V, Cr Mn, Fe and Co (Chemistry of first -row transition elements) in various oxidation states as halides, oxides, hydroxides.

Lanthanoids and Actinoids: (5 h)

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

Bioinorganic Chemistry: (8 h)

Metal ions present in biological systems, classification of elements according to their action in biological system. Geochemical effect on the distribution of metals. Sodium / K-pump, carbonic anhydrase and carboxypeptidase. Excess and deficiency of some trace metals. Toxicity of metal ions (Hg, Pb, Cd and As), reasons for toxicity, Use of chelating agents inmedicine.

Iron and its application in bio-systems, Haemoglobin, Storage and transfer of iron.

Recommended Books:

1. Cotton, F.A., Wilkinson, G. and Gaus, P. L., *Basic Inorganic Chemistry*, 3rd Ed., Wiley, 2007.

2. Huheey, J. E., Keiter, E. A., Keiter, R. L., Medhi, O. K., *Inorganic Chemistry: Principles of Structure and Reactivity*, 4th Ed., Pearson Education India, 2006.

3. Lippard, S.J. & Berg, J.M. *Principles of Bioinorganic Chemistry*, Panima Publishing Company, 1994.

4. Cotton, F.A. & Wilkinson, G, *Advanced Inorganic Chemistry*. 6th Ed., Wiley-VCH, 2007.

5. Basolo, F, and Pearson, R.C., *Mechanisms of Inorganic Chemistry*, John Wiley &Sons, NY, 1967.

6. Greenwood, N.N. &Earnshaw, A., *Chemistry of the Elements*, 2nd Ed., Elsevier India, 2010.

LAB: (30 h)

Gravimetric Analysis:

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

ii. Estimation of copper as CuSCN

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

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

Inorganic Preparations:

i. Tetraamminecopper(II) sulphate, $[Cu(NH_3)_4]SO_4.H_2O$

ii. Cis and trans $K[Cr(C_2O_4)_2.(H_2O)_2]$ Potassium dioxalatodiaquachromate (III)

iii. Tetraamminecarbonatocobalt (III) ion

iv. Potassium tris(oxalato)ferrate(III)

Chromatography of Metal Ions:

Principles involved in chromatographic separations. Paper chromatographic separation offollowing metal ions:

i. Ni(II) and Co(II)

ii. Fe(III) and Al(III)

Recommended Books:

1. Mendham, J. et al.: *Vogel's Textbook of Quantitative Chemical Analysis*; 6th Ed. Pearson Education, 2009.

2. Marr, G. and Rockett, R.W. *Practical Inorganic Chemistry*, Van Nostr and Reinhold. 1972.

3. *Inorganic Syntheses*, Vol. 1-10.

CHE5204C: Organic Chemistry III

Total lectures: 45(L+T) & 30 (P) Credits: 4 (Theory: 03, Lab: 01)

***Course Objectives**: This course introduces students to nucleic acids, amino acids and pharmaceutical compounds. Students will be familiarized with the importance of nucleic acids, amino acids and develop basic understanding of enzymes, bioenergetics and pharmaceutical compounds.*
***Learning Outcome**: Students will be able to explain/describe the important features of nucleic acids, amino acids and enzymes and develop their ability to examine their properties and applications.*

Nucleic Acids , Amino Acids, Peptides and Proteins: (16h)

Components of nucleic acids; Nucleosides and nucleotides;

Polynucleotides: DNA and RNA

Amino acids, Peptides and their classification.

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

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

Enzymes: (8h)

Introduction, classification and characteristics of enzymes. Salient features of active site of enzymes. Mechanism of enzyme action (taking trypsin as example), factors affecting enzyme action, coenzymes and cofactors and their role in biological reactions, specificity of enzyme action (including stereospecificity), enzyme inhibitors and their importance, phenomenon of inhibition (competitive, uncompetitive and non-competitive inhibition including allosteric inhibition).

Lipids: (5h)

Introduction to oils and fats; common fatty acids present in oils and fats, Hydrogenntion of fats and oils, saponification value, acid value, iodine number, rancidity.

Concept of Energy in Biosystems: (8 h)

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

Introduction to metabolism (catabolism, anabolism).

ATP: The universal currency of cellular energy, ATP hydrolysis and free energy change.

Agents for transfer of electrons in biological redox systems: NAD+, FAD.

Conversion of food to energy: Outline of catabolic pathways of carbohydrate- glycolysis, fermentation, Krebs cycle.

Overview of catabolic pathways of fat and protein.

Interrelationship in the metabolic pathways of protein, fat and carbohydrate.

Recommended Books:

1. Berg, J.M., Tymoczko, J.L. and Stryer, L. (2006) *Biochemistry*. VIth Edition. W.H. Freeman and Co.
2. Nelson, D.L., Cox, M.M. and Lehninger, A.L. (2009) *Principles of Biochemistry*. IV Edition. W.H. Freeman and Co.

3. Murray, R.K., Granner, D.K., Mayes, P.A. and Rodwell, V.W. (2009) Harper's *Illustrated Biochemistry*. XXVIII edition. Lange Medical Books/ McGraw-Hill

LAB: (**30 h)**

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

9. Estimation of glucose

Recommended Books:

1. Arthur, I. V. *Quantitative Organic Analysis,* Pearson.
2. Plummer, D. T. *An Introduction to Practical Biochemistry*, 3rd Edition, McGraw Hill.

CHE5304C: Physical Chemistry-II

Total lectures: 45(L+T) & 30 (P) Credits: 4 (Theory: 03, Lab: 01)

Course Objective: *The aim of this course is to teach students four important topics of physical chemistry- chemical kinetics, catalysis, photochemistry and surface chemistry. Chemical kinetics and conductance will be discussed in detail but photochemistry, surface chemistry and catalysis will be introduced to the students.*

Learning Outcome: *The students are expected to learn rate laws of chemical transformation, experimental methods of rate law determination, steady state approximation etc. in chemical kinetics unit. After attending this course the students will be able to understand different types of surface adsorption processes, photochemical phenomena, conductometric titration and basics of catalysis including enzyme catalysis, acid base catalysis and particle size effect on catalysis.*

Chemical Kinetics & Catalysis: (23 h)

Order and molecularity of a reaction, rate laws in terms of the advancement of a reaction, differential and integrated form of rate expressions up to second order reactions, experimental methods of the determination of rate laws, kinetics of complex reactions (integrated rate expressions up to first order only): (i) Opposing reactions (ii) parallel reactions and (iii) consecutive reactions and their differential rate equations (iv) chain reactions. Temperature dependence of reaction rates; Arrhenius equation; activation energy. Collision theory of reaction rates, Lindemann mechanism, qualitative treatment of the theory of absolute reaction rates. Reaction mechanism- steady-state approximation and rate determining step approximation methods.

Types of catalyst, specificity and selectivity, mechanisms of catalyzed reactions at solid surfaces; effect of particle size and efficiency of nanoparticles as catalysts. Enzyme catalysis, Michaelis-Menten mechanism, acid-base catalysis.

Photochemistry: (7 h)

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

Surface Chemistry: (5 h)
Physical adsorption, chemisorption, adsorption isotherms, nature of adsorbed state.

Ionic motion in liquid: (10 h)

Ionic velocities, mobilities and their determinations, transference numbers and their relation to ionic mobilities, determination of transference numbers using Hittorf and Moving Boundary method. Applications of conductance measurement: (i) degree of dissociation of weak electrolytes, (ii) ionic product of water (iii) solubility and solubility product of sparingly soluble salts, (iv) conductometric titrations, and (v) hydrolysis constants of salts.

Recommended Books:

1. Peter Atkins & Julio De Paula, *Physical Chemistry 9th Ed.,* Oxford University Press (2010).
2. Castellan, G. W. *Physical Chemistry,* 4th Ed., Narosa (2004).
3. Engel, T. & Reid, P. *Physical Chemistry 3rd Ed.,* Prentice-Hall (2012).
4. Zundhal, S.S. *Chemistry concepts and applications* Cengage India (2011).
5. Ball, D. W. *Physical Chemistry* Cengage India (2012).
6. Mortimer, R. G. *Physical Chemistry 3rd Ed.,* Elsevier: NOIDA, UP (2009).
7. Levine, I. N. *Physical Chemistry 6th Ed.,* Tata McGraw-Hill (2011).
8. Metz, C. R. *Physical Chemistry 2nd Ed.,* Tata McGraw-Hill (2009).

LAB: (30h)

Chemical Kinetics
Study the kinetics of the following reactions.
1. Initial rate method: Iodide-persulphate reaction
2. Integrated rate method:
    a. Acid hydrolysis of methyl acetate with hydrochloric acid.
    b. Saponification of ethyl acetate.
3. Compare the strengths of HCl and H_2SO_4 by studying kinetics of hydrolysis of methyl acetate.

Adsorption
1.Verify the Freundlich and Langmuir isotherms for adsorption of acetic acid on activated charcoal.

Conductometry
I. Determination of cell constant
II. Determination of equivalent conductance, degree of dissociation and dissociation

constant of a weak acid.
III. Perform the following conductometric titrations:
i. Strong acid vs. strong base
ii. Weak acid vs. strong base
iii. Mixture of strong acid and weak acid vs. strong base
iv. Strong acid vs. weak base

Recommended Books:
1. Khosla, B. D.; Garg, V. C. & Gulati, A., *Senior Practical Physical Chemistry,* R. Chand & Co.: New Delhi (2011).
2. Athawale, V. D. & Mathur, P. *Experimental Physical Chemistry* New Age International: New Delhi (2001).
3. Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. *Experiments in Physical Chemistry 8th Ed.;* McGraw-Hill: New York (2003).
4. Halpern, A. M. & McBane, G. C. *Experimental Physical Chemistry 3rd Ed.;* W.H. Freeman & Co.: New York (2003).

CHE5404C: Quantum Chemistry-I

Total lectures: 45(L+T) & 30 (P) Credits: 4 (Theory: 03, Lab: 01)

Course Objective: *The aim of this course is to introduce the students with two important areas- quantum chemistry and chemical bonding. In quantum chemistry unit the students will be taught the postulates of quantum mechanics and the application of quantum mechanical ideas in some simple systems such as particle in a box, rigid rotor, simple harmonic oscillator etc.*

Learning Outcome: *After completion of this course the students are expected to understand the foundation of quantum mechanics and its application in some simple chemical systems such as hydrogen atom or hydrogen like ions. The students will also learn chemical bonding in some simple molecular systems.*

Postulates of Quantum Mechanics: (6 h)

Postulates of quantum mechanics, quantum mechanical operators, Schrödinger equation.

Models in Quantum Chemistry: (14 h)

Free particle and "particle-in-a-box" (rigorous treatment), quantization of energy levels, zero-point energy Extension to two and three dimensional boxes, separation of variables, degeneracy. Qualitative treatment of simple harmonic oscillator model of vibrational motion: Setting up of Schrödinger equation and discussion of solution and wavefunctions. Vibrational energy of diatomic molecules and zero-point energy.

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

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

Structure of One-Electron Systems: (5 h)

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

Chemical Bonding: (20 h)

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

Covalent bonding, valence bond and molecular orbital approaches, LCAO-MO treatment of H_2^+. Bonding and antibonding orbitals. Qualitative extension to H_2. Comparison of LCAO-MO and VB treatments of H2 (only wavefunctions, detailed solution not required) and their limitations. Refinements of the two approaches (Configuration Interaction for MO, ionic terms in VB). Qualitative description of LCAO-MO treatment of homonuclear and heteronuclear diatomic molecules (HF, LiH). Localised and non-localised molecular orbitals treatment of triatomic (BeH_2, H_2O) molecules. Qualitative MO theory and its application to AH_2 type molecules.

Recommended Books:

1. McQuarrie, D. A. *Quantum Chemistry*, Viva Books (2016)
2. Chandra, A. K. *Introductory Quantum Chemistry* Tata McGraw-Hill (2001).
3. House, J. E. *Fundamentals of Quantum Chemistry 2nd Ed*. Elsevier: USA (2004).
4. Lowe, J. P. & Peterson, K. *Quantum Chemistry*, Academic Press (2005).
5. Sen, B. K. *Quantum Chemistry- Including Spectroscopy*, Kalyani Publishers; 4th edition (2011).
6. Kapoor, K. L. *A Textbook of Physical Chemistry (Volume 4)* McGraw Hill Education; 5th edition (2017).
7. Kakkar, R. *Atomic & Molecular Spectroscopy*, Cambridge University Press (2015).
8. Banwell, C. N. &McCash, E. M. *Fundamentals of Molecular Spectroscopy 4th Ed*. Tata McGraw-Hill: New Delhi (2006).

LAB: (30 h)

1. Introduction to open-source computational chemistry tools
2. Molecular modeling
3. Single-point energy calculation of chemical systems in their ground and excited electronic states
4. Geometry optimization of molecules
5. Energy calculations of conformers
6. Energy calculation of molecules in solvent system (discrete)

Recommended Books:

1.Lewars, E. *Computational Chemistry*, (Springer, 2003).

CHE6104C: Inorganic Chemistry-III

Total lectures: 45(L+T) & 30 (P) Credits: 4 (Theory: 03, Lab: 01)

Course Objective: *The unit on reaction mechanism is included for the students to get acquainted with the kinetic and thermodynamic factors governing the reaction path and stability of inorganic compounds. Organometallic compounds are introduced so as to apprise students about the importance of metal carbon bond to form complexes and their application as catalysts. Students are expected to learn factors leading to stability of organometallic compounds, their synthesis, reactivity and uses. Qualitative inorganic analysis is included to give students an idea and hands on experience of application of inorganic chemistry. Students should learn how differential reactivity under different conditions of pH can be used to identify variety of ions in a complex mixture. Experiments related to synthesis and characterization of coordination compounds are included to supplement their theoretical knowledge.*

Learning Outcome: *By studying this course the students will be expected to learn about how ligand substitution and redox reactions take place in coordination complexes. Students will also learn about organometallic compounds, comprehend their bonding, stability, reactivity and uses. They will be familiar with the variety of catalysts based on transition metals and their application in industry. On successful completion, students in general will be able to appreciate the use of concepts like solubility product, common ion effect, pH etc. in analysis of ions and how a clever design of reactions, it is possible to identify the components in a mixture. With the experiments related to coordination compound synthesis, calculation of 10Dq, controlling factors etc. will make the students appreciate the concepts of theory in experiments.*

Mechanism of Inorganic Reactions: (12 h)

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

Organometallic Compounds: (18 h)

Definition and classification of organometallic compounds on the basis of bond type. Concept of hapticity of organic ligands.

Metal carbonyls: 18 electron rule, electron count of mononuclear, polynuclear and substituted metal carbonyls of 3d series. General methods of preparation (direct combination, reductive carbonylation, thermal and photochemical decomposition) of mono and binuclear carbonyls of 3d series. Structures of mononuclear and binuclear carbonyls of Cr, Mn, Fe, Co and Ni using VBT. Π-acceptor behaviour of CO

(MO diagram of CO to be discussed), synergic effect and use of IR data to explain extent of back bonding. Zeise's salt: Preparation and structure, evidences of synergic effect and comparison of synergic effect with that in carbonyls.

Metal Alkyls: Important structural features of methyl lithium (tetramer) and trialkylaluminium (dimer), concept of multicentre bonding in these compounds. Role of triethylaluminium in polymerisation of ethene (Ziegler – Natta Catalyst). Species present in ether solution of Grignard reagent and their structures, Schlenk equilibrium. Ferrocene: Preparation and reactions (acetylation, alkylation, metallation, Mannichcondensation). Structure and aromaticity. Comparison of aromaticity and reactivity with that of benzene.

Transition Metals in Catalysis: (8 h)

Study of the following industrial processes and their mechanism:

1. Alkene hydrogenation (Wilkinson's Catalyst)

2. Hydroformylation (Co catalysts)

3. Wacker Process

4. Synthetic gasoline (Fischer Tropsch reaction)

5. Synthesis gas by metal carbonyl complexes

Theoretical Principles in Qualitative Inorganic Analysis (H_2S Scheme): (7 h)

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

Recommended Books:

1. Vogel, A.I. *Qualitative Inorganic Analysis*, Longman, 1972.

2. Svehla, G. &Sivasankar, B., *Vogel's Qualitative Inorganic Analysis*, 7th Ed., Prentice Hall, 2012.

3. Cotton, F.A., Wilkinson, G. and Gaus, P. L., *Basic Inorganic Chemistry*, 3rd Ed.,Wiley, 2007.

4. Cotton, F.A. & Wilkinson, G, *Advanced Inorganic Chemistry*. 6th Ed., Wiley-VCH, 2007.

5. Huheey, J. E., Keiter, E. A., Keiter, R. L., Medhi, O. K., *Inorganic Chemistry: Principles of Structure and Reactivity*, 4th Ed., Pearson Education India, 2006.

6. Sharpe, A.G. *Inorganic Chemistry*, 4th Indian Reprint (Pearson Education) 2005

7. Douglas, B.E. and Mc Daniel, D.H., *Concepts and Models of Inorganic Chemistry*, 3rdEd. Wiley India, 2006.

8. Greenwood, N.N. &Earnshaw, A., *Chemistry of the Elements*, 2nd Ed., Elsevier India, 2010.

9. Lee, J. D., *Concise Inorganic Chemistry*, 5th Ed., Oxford University Press, 2008.

10. Powell, P. *Principles of Organometallic Chemistry*, Chapman and Hall, 1988.

11. Shriver, D.D. & Atkins, P., *Inorganic Chemistry 2nd Ed*., Oxford University Press, 1994.

12. Basolo, F. & Person, R. *Mechanisms of Inorganic Reactions: Study of Metal Complexes in Solution 2nd Ed..*, John Wiley & Sons Inc; NY.

13. Purcell, K.F. &Kotz, J.C., *Inorganic Chemistry*, W.B. Saunders Co. 1977

14. Miessler, G. L. &Tarr, D. A., *Inorganic Chemistry 4th Ed.*, Pearson, 2010.

15. Crabtree, Robert H. *The Organometallic Chemistry of the Transition Metals*. New York, NY: John Wiley, 2000.

16. Spessard, Gary O., &Gary L. Miessler. *Organometallic Chemistry*. Upper Saddle River, NJ: Prentice-Hall, 1996.

LAB: (30 h)

- Qualitative semimicro analysis of mixtures containing 3 anions and 3 cations. Emphasis should be given to the understanding of the chemistry of different reactions. The following radicals are suggested: CO_3^{2-} , NO_2^- , S_2^- , SO_3^{2-}, $S_2O_3^{2-}$, CH_3COO^- , F^- , Cl^- , Br^- , I^- , NO_3^- , BO_3^{3-} , $C_2O_4^{2-}$, PO_4^{3-} , NH_4^+ , K^+ , Pb^{2+}, Cu^{2+}, Cd^{2+}, Bi^{3+}, Sn^{2+}, Sb^{3+}, Fe^{3+}, Al^{3+},, Cr^{3+}, Zn^{2+} , Mn^{2+}, Co^{2+}, Ni^{2+}, Ba^{2+} , Sr^{2+}, Ca^{2+}, Mg^{2+}

- Mixtures should preferably contain one interfering anion, or insoluble component ($BaSO_4$, $SrSO_4$, $PbSO_4$, CaF_2 or Al_2O_3) or combination of anions e.g. CO_3^{2-} and SO_3^{2-} , NO_2 and NO_3^- , Cland Br^- , Cland I^- , Brand I^- , NO_3^- and Br^- , NO_3^- and I^- .

- Spot tests should be done whenever possible.

- Synthesis of ammine complexes of Ni(II) and their ligand exchange reactions involving bidentate ligands like acetylacetone, dimethylglyoxime, glycine, etc.

- Preparation of acetylacetanato complexes of Cu^{2+}/Fe^{3+} .

- Controlled synthesis of two copper oxalate hydrate complexes: kinetic vs. thermodynamic factors.

- Determination of εmax value from UV-visible spectra of complexes.

- Measurement of 10 Dq by spectrophotometric method, verification of spectrochemical series.

Recommended Books:

1. *Vogel's Qualitative Inorganic Analysis*, Revised by G. Svehla.

2. Marr, G. and Rockett, R.W. *Practical Inorganic Chemistry*, Van Nostrand Reinhold. 1972.

CHE6204C: Organic Chemistry-IV

Total lectures: 45(L+T) & 30 (P) Credits: 4 (Theory: 03, Lab: 01)

Course Objectives*: This is a basic course in organic reagents and provides introduction to carbohydrate chemistry, dyes and polymers. Students are expected to learn about the different oxidizing and reducing agents and their applications in organic chemistry. Students shall be apprised with carbohydrate chemistry, dyes and polymers and their structure, reactivity and chemical properties.*

Learning Outcome*: Students will be able to explain/describe basic principles of different reagents and their importance in chemical/organic synthesis. Students shall be able to classify/identify/critically examine carbohydrates, polymers and dye materials.*

Oxidation Reactions: (10 h)

Metal based and non-metal based oxidations (Cr, Mn, Al, Ag, Os, Ru, Se, DMSO, hypervalent iodine and TEMPO based reagents). Reagents (Fremy's salt, silver carbonate, peroxides/per-acids). Sharpless asymmetric epoxidation, Jacobsen epoxidation, Shi epoxidation, Sharpless asymmetric dihydroxylation, Baeyer-Villiger oxidation, Wacker oxidation, hydroboration-oxidation, Prevost reaction and Woodward modification.

Reduction Reactions: (12 h)

Catalytic hydrogenation (Pd/Pt/Rh/Ni). Wilkinson catalyst, Noyori asymmetric hydrogenation, Metal based reductions using Li/Na/Ca in liquid ammonia, Sodium, Magnesium, Zinc, Titanium and Samarium (Birch, Pinacol formation, McMurry, Acyloin formation, dehalogenation and deoxygenations); Hydride transfer reagents from Group III and Group IV in reductions (NaBH4 triacetoxyborohydride, L-selectride, K-selectride, Luche reduction, LiAlH4, DIBAL-H, and Red-Al, Trialkylsilanes and Trialkylstannane, Meerwein-Pondorff-Verley reduction); Stereo/enantioselective reductions (Chiral Boranes, Corey-Bakshi-Shibata).

Carbohydrates: (9h)

Occurrence, classification and their biological importance.

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

Disaccharides – Structure elucidation of maltose, lactose and sucrose.

Polysaccharides – Elementary treatment of starch, cellulose and glycogen.

Alkaloids and Terpenes: (14h)

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

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

Recommended Books:

LAB: (30 h)

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

Recommended Books:

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

CHE6304C: Physical Chemistry-III

Total lectures: 45(L+T) & 30 (P) Credits: 4 (Theory: 03, Lab: 01)

Course Objective: *The aim of this course is to introduce students with phase equilibrium and its applications, electrochemistry, polymer chemistry and electrical and magnetic properties of chemical systems.*

Learning Outcome: *In this course the students will learn theories of phase equilibria and electrochemistry. The students are also expected to understand the various parts of electrochemical cells along with Faraday's Laws of electrolysis. The students will also gain basic theoretical idea of polymers and electrical & magnetic properties of atoms and molecules.*

Phase Equilibria: (18 h)

Concept of phases, components and degrees of freedom, derivation of Gibbs Phase Rule for nonreactive and reactive systems; Clausius-Clapeyron equation and its applications to solid-liquid, liquid-vapour and solid-vapour equilibria, phase diagram for one component systems, with applications. Phase diagrams for systems of solid-liquid equilibria involving eutectic, congruent and incongruent melting points, solid solutions.

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

Nernst distribution law: its derivation and applications.

Electrochemistry: (12 h)

Quantitative aspects of Faraday's laws of electrolysis, rules of oxidation/reduction of ions based on half-cell potentials. Chemical cells, reversible and irreversible cells with examples. Electromotive force of a cell and its measurement, Nernst equation; Standard electrode (reduction) potential and its application to different kinds of half-cells. Application of EMF measurements in determining (i) free energy, enthalpy and entropy of a cell reaction, (ii) equilibrium constants, and (iii) pH values, using hydrogen, quinone-hydroquinone, glass and SbO/Sb_2O_3 electrodes. Concentration cells with and without transference, liquid junction potential; determination of activity coefficients and transference numbers. Qualitative discussion of potentiometric titrations (acid-base, redox, precipitation). Applications of electrolysis in metallurgy and industry.

Electrical & Magnetic Properties of Atoms and Molecules: (7 h)

Basic ideas of electrostatics, Electrostatics of dielectric media, Clausius-Mosotti equation, Lorenz-Laurentz equation, Dipole moment and molecular polarizabilities and their measurements. Diamagnetism, paramagnetism, magnetic susceptibility and its measurement, molecular interpretation.

Polymer Chemistry: (8 h)

Molecular weight of polymers, determination of molecular weight, molecular weight distribution and its significance, polydispersity index, kinetics of polymerization reaction, copolymerization, average dimension of polymer molecules, size exclusion chromatography.

Recommended Books:

1. Atkins, P.W & Paula, J.D. *Physical Chemistry*, 9th Ed., Oxford University Press (2011).
2. Castellan, G. W. *Physical Chemistry 4th Ed.*, Narosa (2004).
3. Mortimer, R. G. *Physical Chemistry 3rd Ed.*, Elsevier: NOIDA, UP (2009).
4. Barrow, G. M., *Physical Chemistry 5th Ed.*, Tata McGraw Hill: New Delhi (2006).
5. Engel, T. & Reid, P. *Physical Chemistry 3rd Ed.*, Prentice-Hall (2012).
6. Rogers, D. W. *Concise Physical Chemistry* Wiley (2010).
7. Silbey, R. J.; Alberty, R. A. &Bawendi, M. G. *Physical Chemistry 4th Ed.*, John Wiley & Sons, Inc. (2005).
8. Puri, B. R.; Sharma, L. R.; Pathania, M. S. *Principles of Physical Chemistry*, Vishal Publishing Co.; 47th Ed. (2017).
9. Kapoor, K. L. *A Textbook of Physical Chemistry (Volume 1)* McGraw Hill Education; Sixth edition (2019).

10. Gowarikar, V. R.; Viwanathan, N. V.; Sreedhar, J. *Polymer Science*, 1st Edition, New age International Publishers (1986).
11. G. Odian, *Principles of Polymerization*, 4th Edition, Willy Student Edition (2004).

LAB: **(30h)**

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

II. Phase equilibria: Construction of the phase diagram using cooling curves or ignition tube method:
a. simple eutectic and
b. congruently melting systems.

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

IV. Study the equilibrium of at least one of the following reactions by the distribution method:
(i) $I_2(aq) + I \rightarrow I_3(aq)2+$
(ii) $Cu^{2+}(aq) + nNH_3 \rightarrow Cu(NH_3)n$

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

CHE6404C: Spectroscopy-I

Total lectures: 45(L+T) & 30 (P) Credits: 4 (Theory: 03, Lab: 01)

Course Objective: *The aim of this course is to introduce the students with important areas of molecular spectroscopy and its application. In spectroscopy unit, rotational, vibrational, Raman, electronic, spin resonance, and electronic spectroscopy will be introduced.*
Learning Outcome: *After completion of this course the students are expected to understand the application of various kinds of spectroscopic techniques.*

Introduction to Molecular Spectroscopy: **(5 h)**

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

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

Vibrational Spectroscopy: (15 h)

Classical equation of vibration, computation of force constant, amplitude of diatomic molecular vibrations, anharmonicity, Morse potential, dissociation energies, fundamental frequencies, overtones, hot bands, degrees of freedom for polyatomic molecules, modes of vibration, concept of group frequencies. Vibration-rotation spectroscopy: diatomic vibrating rotator, P, Q, R branches. Fundamental and non-fundamental molecular vibrations; IR absorption positions of O, N and S containing functional groups; Effect of H-bonding, conjugation, resonance and ring size on IR absorptions; Fingerprint region and its significance; application in functional group analysis.

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

Electronic Spectroscopy: (15 h)

Franck-Condon principle, electronic transitions, singlet and triplet states, fluorescence and phosphorescence, dissociation and predissociation, calculation of electronic transitions of polyenes using free electron model.Types of electronic transitions, λmax, Chromophores and Auxochromes, Bathochromic and Hypsochromic shifts, Intensity of absorption; Application of Woodward Rules for calculation of λmax for the following systems: α,βunsaturated aldehydes, ketones, carboxylic acids and esters; Conjugated dienes: alicyclic,homoannular and heteroannular; Extended conjugated systems (aldehydes, ketones and dienes); distinction between cis and trans isomers.

NMR and ESR Spectroscopy: (10 h)

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

Electron Spin Resonance spectroscopy: Its principle, hyperfine structure, ESR of simple radicals.

Applications of IR, UV and NMR for identification of simple organic and inorganic molecules.

Recommended Books:

1. Banwell, C. N. &McCash, E. M. *Fundamentals of Molecular Spectroscopy* 4th Ed. Tata McGraw-Hill: New Delhi (2006).
2. Kakkar, R. *Atomic & Molecular Spectroscopy*, Cambridge University Press (2015).
3. *Introduction to Spectroscopy* by D. L. Pavia; G. M. Lampman and G. S. Kriz

LAB: (30 h)

UV/Visible Spectroscopy

1. Study the 200-500 nm absorbance spectra of KMnO4 and K2Cr2O7 (in 0.1 M H2SO4) and determine the λmaxvalues. Calculate the energies of the two transitions in different units (J molecule^{-1}, kJ mol-1, cm^{-1}, eV).

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

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

4. Verify Lambert-Beer's law and determine the concentration of

$CuSO_4$/$KMnO_4$/$K_2Cr_2O_7$in a solution of unknown concentration

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

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

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

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

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

10. Analysis of the given vibration-rotation spectrum of HCl(g)

Recommended Books:

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

CHE7104C: Inorganic Chemistry-IV

Total lectures: 45(L+T) & 30 (P) Credits: 4 (Theory: 03, Lab: 01)

Course Objective: *This is an introductory course on inorganic chemistry, through which students will appreciate the chemistry of the transition metals, aspects related tobonding, oxidation states and electronic/magnetic properties.*

Learning Outcome: *Students will be able to explain/critically examine the chemistry of transition metals, structure and bonding.*

Descriptive Inorganic Chemistry: (23 h)

Structure and bonding in polyhedral boranes and carboranes, electron count in polyhedral boranes – styx numbering, Wade's rules – polyhedral skeletal electron pair theory (PSEPT), synthesis of polyhedral boranes. Metal borides.

Organo compounds of Si, Ge, Sn and Pb; phosphates, phosphazenes and phosphines; metal-oxo compounds, calixarenes, cryptands and crown ethers in complexation chemistry, metal chalcogenides, sulfur-nitrogen compounds

Organometallic compounds of Li, Be, Mg and Hg

Chemistry of the elements of the second and third transition series – general overview of compounds having the metals in their common oxidation states; polyoxometallates of Mo and W; quadruple and quintuple M-M bonded compounds, methyltrioxorhenium (MTO); the Creutz-Taube complex; RuCl2(PPh3)3; osmium tetroxide; Vaska‘s compound; palladium complexes in the oxidation state 0; Pt(II,IV) linear chain compounds.

Nuclear and Radiochemistry: (12 h)

Radioactive decay processes, Fermi theory, half-lives, auger effect. Nuclear reactions – notations, comparison with chemical reaction: Types of nuclear reactions. Applications of radioisotopes as tracers (activation and isotope dilution analysis). Age determination, radiolysis of water, units for measuring radiation absorbed by matter, radiation dosimetry. Radiation induced chemistry–sources of radiation, chemical effects produced by the absorption of ionizing radiation and high energy ions and electrons from accelerators - radiation induced synthesis of materials.

Organometallic Chemistry-II: (10 h)

Synthesis, structure, bonding and reactivity of mono and polynuclear metal carbonyls. Substituted metal carbonyls. Vibrational spectra of metal carbonyls.

Types of M-C bonds, synthesis and reactivity of metal alkyls, carbenes, alkenes, alkynes, and arene complexes; metallocenes and bent metallocenes.

Recommended Books:

1. F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann; *Advanced Inorganic Chemistry*, 6th ed. Wiley, 1999

2. P.W. Atkins, T. Overton, J. Rourke, M. Weller, F. Armstrong; *Shriver & Atkins‘ Inorganic Chemistry*, 5th ed. Oxford University Press, 2010.

3. *Fundamental Concepts of Inorganic Chemistry*, Vols. 1-7, by A.K. Das and M. Das, CBS Publishers and Distributors, 2015

4. L. Smart, E. Moore, *Solid State Chemistry: An Introduction*, 2nd Ed. Nelson Thorns Ltd. 2004.

5. A. R. West, *Solid State Chemistry and Its Application*, Wiley Student Edition, John Wiley & Sons. 1998.

6. R. H. Crabtree, *Organometallic Chemistry of the Transition Metals 2nd Ed*., John Wiley, 1993.

7. C.Elschenbroich, A. Salzer, *Organometallics: A Concise Introduction*, 2nd Ed. Wiley VCH, 1995.

LAB: (30 h)

1. Solid phase synthesis of coordination compounds (e.g. Reinecke salt, trans-bis-glycinatocopper(II)) and their properties.

2. Synthesis of metal nanoparticles (Cu, Ag, Au, etc.), characterization and investigation of their optical properties.

CHE7204C: Organic Chemistry-V

Total lectures: 45(L+T) & 30 (P) Credits: 4 (Theory: 03, Lab: 01)

Course objective: *Students will be introduced to the concepts of reaction mechanism, reaction intermediates and stereochemistry.*
Learning outcome: *Students will be able to appreciate/demonstrate/explain the unique features of organic reactions mechanism, reaction intermediates and stereochemistry, and solve related problems*

Kinetics and Energetics of Reaction Mechanism: (13h)

TST theory of reaction rates: kinetics & thermodynamics of activation. Reaction profiles for multistep reactions, Hammond postulate, Curtin-Hammett Principle; kinetic and thermodynamic control.

Linear free energy relationships (LFER): Hammett equation - substituent and reaction constants; the Taft treatment of polar and steric effects in aliphatic compounds; kinetic isotope effects in organic reactions.

Effects of conformation on reactivity: anomeric effect, stereoelectronic effects, neighbouring group participation.

Reaction Mechanisms & Intermediates: Structure & Reactivity-I: (12h)

Carbanions: enolates and enamines, Kinetic and thermodynamic enolates, lithium and boron enolates in aldol and Michael reactions, alkylation and acylation of enolates; name reactions under carbanion chemistry - Claisen, Dieckmann, Knoevenegal, Stobbe, Darzen, Acyloin condensations, Shapiro reaction, Julia olefination,

Brook rearrangement,Sakuraireaction,Henryreaction,Kulinkovichreaction,Nefreaction,Baylis-Hillman reaction

Ylids: Chemistry of phosphorous and sulfur ylids-Wittig and related reactions, Peterson olefination

Reaction Mechanisms &Intermediates: Structure & Reactivity-II: (10 h)

Carbenes and Nitrenes: Structure of carbenes, generation of carbenes, addition and insertion reactions, rearrangement reactions of carbenes such as Wolff rearrangement, generation and reactions of ylids by carbenoid decomposition (existence of O and N based ylids), Structure of nitrene, generation and

reactions of nitrene and related electron deficient nitrogen intermediates, Curtius, Hoffmann, Schmidt, Beckmann rearrangement, Tebbeolefination reactions.

Radicals: Generation of radical intermediates and its (a) addition to alkenes, alkynes (inter &intramolecular) for C-C bond formation and Baldwin‘s rules (b) fragmentation and rearrangements. Name reactions involving radical intermediates such as Barton deoxygenation and decarboxylation, McMurry coupling.

Stereochemistry: (10h)

Classification of organic molecules into different Point Groups, R/S, E/Z nomenclature in C, N, S, P containing compounds; concept of absolute and relative configuration; chirality in molecules devoid of chiral centers- allenes, spiranes and biphenyls (atropisomerism).

Concepts of stereogenic center – chirotopic and achirotopic center; homotopic and heterotopic ligands and faces (prostereoisomerism and prochiralityetc); optical purity and enantiomeric excess; conformation of acyclic organic molecules, cyclohexane and decalins.

Recommended Books:

1. F. A. Cary and R. I. Sundberg, *Advanced Organic Chemistry*, Part A and B, 5th Edition, Springer, 2009.
2. A. J. Kirby, *Stereoelectronic Effects*, 1st edition, OUP
3. T. H. Lowry, K. S. Richardson, *Mechanism and Theory in Organic Chemistry*.
4. J. Clayden, N. Greeves, S. Warren, *Organic Chemistry*, 2nd edition, OUP 2012
5. E. V. Anslyn, D. A. Dougherty, *Modern Physical Organic Chemistry*, University Science Books, 2005
6. E.L. Eliel, S. H. Wilen, *Stereochemistry of Organic Compounds*

LAB: (30 h)

Qualitative analysis: Binary mixture analysis (solid-solid, solid-liquid, liquid-liquid)

Experiments on Natural products:

Introduction to extraction and phytochemical screening/analysis of Natural Products (A case study).

Extraction of carotenoids from a natural source.

Isolation of (−)-Menthol from Peppermint Oil.

Saponification of Vegetable Oil

Conversion of Vegetable Oil to Biodiesel.

Recommended Books:

1. B. S. Furniss, A. J. Hannaford, P. W. G. Smith, *Vogel‘s Textbook of Practical Organic Chemistry*, Pearson, 2012.
2. V. K. Ahluwalia, S. Dhingra, *Comprehensive Practical Organic Chemistry*, University Press.
3. F. G. Mann, B. C. Saunders, *Practical Organic Chemistry*, 3rd Edition Longman, 1978
4. Selected articles from *Journal of Chemical Education*, ACS Publications.

CHE7304C: Physical Chemistry-IV

Total lectures: 45(L+T) & 30 (P) Credits: 4 (Theory: 03, Lab: 01)

Course Objective: *The aim of this course is to introduce students with non- equilibrium thermodynamics, statistical thermodynamics and approximation methods of quantum chemistry.*
Learning Outcome: *In this course the students will learn theories of non- equilibrium thermodynamics and statistical thermodynamics, the students are also expected to understand the various approximation methods Quantum Chemistry. The students will also gain knowledge on application of quantum mechanics in thermodynamics.*

Equilibrium and Non-Equilibrium Thermodynamics: (10 h)

Laws of thermodynamics, state and path functions and their applications, Maxwell's relations; spontaneity and equilibria; Le Chatelier principle, non-ideal system: thermodynamics of real gases and gas mixtures, fugacity and its determination, non-ideal solutions, activity and activity coefficient-different scales of activity coefficient, electronic activity coefficients, phase equilibrium: thermodynamic criteria of phase equilibrium, Gibbs phase rule and its application to three component systems- triangular plots- water- acetic acid –chloroform system, ammonium chloride-ammonium sulphate-water system, non-equilibrium thermodynamics: forced flows and entropy of production, coupled flows and phenomenological relations, Onsager reciprocal relations, thermodynamic effects- Seebeck and Peltier and Thomson effect.

Statistical Thermodynamics: (12 h)

Statistical mechanics of systems independent particles: Maxwell Boltzmann distribution, entropy and probability. Calculation of thermodynamic properties for independent particles,- molecular partition functions- evaluation of translational, rotational and vibrational and nuclear partition functions, thermodynamic properties of monatomic and diatomic gases (Suckur-Tetrode equation)- calculation of partition functions, thermodynamic function, principles of equipartition, heat capacities (Einstein model and Debye modification), residual entropy, equilibrium constant

Approximate Methods: (12 h)

Time-independent perturbation theory of a two-level system (up to second order), the first order correction to the energy and wave function, perturbation theory for degenerate states, the second order correction to the energy, time dependent behaviour of a two level system, the Rabi formula, the effect of a slowly switched constant perturbation, the variation theorem, linear variation function-secular equation, the Rayleigh ratio.

Born-Oppenheimer Approximation: (11 h)

Born-Oppenheimer approximation, product wave-functions, complete many electron wave functions including electron spin, Pauli's anti-symmetry and exclusion principles, Singlet and triplet states, central field model of many electron atoms (He atom), Slater type orbitals, splitting of term energies in presence of electric and magnetic field (Stark effect and Zeeman effect)

Recommended Books:

1. Atkins, P; Paula, J. *Physical Chemistry*, 9th Edition, Oxford University Press, Oxford 2010.

2. Levine, I. R. *Physical Chemistry*, 6th Edition, Mcgraw Hill Education, 2011.

3. McQuarrie, D. A; Simon, J. D. *Physical Chemistry: A Molecular Approach*, Viva Student Edition, 1st Edition, 2011.

4. Berry, R. S.; Rice, S. A.; Ross, J. *Physical Chemistry*, 2nd Edition, Oxford University Press, Oxford 2007.

5. McQuarrie, D. A. *Statistical Mechanics*, University Science Books, California, 2005.

6. Atkins, P.; Friedman, R. *Molecular Quantum Mechanics*, 4th Edition, Oxford University Press, Oxford 2008.

7. Levine, I. N. *Quantum Chemistry*, 7th Edition, PHI Learning Pvt. Ltd., 2014.

8. David J. Griffiths, *Introduction to Quantum mechanics*, 2nd edition, Pearson Education Ltd., 2014

9. Szaboo A., Ostlund N. S., *Modern Quantum Chemistry*, 1st edition (Revised), 2015.

LAB: **(30h)**

Exercise:

i. Construction of Z-matrix for H_2CO

ii. Construction of Z-matrix for H_2CO with molecular symmetry

iii. Construction of Z-matrix using molecular symmetry for CH_3OH

iv. Construction of Z-matrix using molecular symmetry for CH_4

v. Construction of Z-matrix using a dummy atom for CO_2

vi. Reading and interpreting output of GAMESS, dissociation energy of H_2O.

vii. Examples for EHT including Walsh diagram for simple molecules

Recommended Books

1. Lewars, E. *Computational Chemistry*, (Springer, 2003).

2. Balagurusamy, E. *Numerical Methods*, (Tata McGraw-Hill Publishing Company Limited, 2002

CHE7404C: Research Methodology

Total lectures: 45(L+T) & 30 (P) Credits: 4 (Theory: 03, Lab: 01)

Course Objective*:This course will introduce students with the basic principles of chemical research.*

***Learning Outcome**s:On completion of this course the students will be able to learn application of a number of principles as applied to chemical research; design, conduct, analyse and interpret results of an experiment, and effectively communicate these in written reports; critical analysis and evaluation of quantitative & qualitative chemical information; obtain and evaluate information from a variety of sources.*

Introduction to Research Methodology: (12h)

Research Methodology: An Introduction,Objectives of Research, Types of Research, defining a Research Problem, Techniques involved in Defining a Problem Research Design TechnicalWriting, Ethics in Research, Software for Plagiarism.

Error Analysis: (5h)

Instrumental and statistical uncertainties, propagation of errors, specific error formulae, application of error equation.

Hypothesis and Research Methodology: (18h)

Basic Principles of Experimental Designs and Sampling, Methods of Data Collection and Analysis Collection of Primary and Secondary Data, Selection of appropriate method Data Processing Operations, Elements of Analysis, Statistics in Research, Regression Analysis, Correlation Techniques of Hypotheses, Parametric or Standard Tests Basic concepts.

Computational Techniques: (10h)

Analysis of Variance and Co-variance ANOVA, One way ANOVA, Two Way ANOVA, ANOCOVA, Assumptions in ANOCOVA, Basics of computational chemistry.

Recommended Books:

1. Kothari, C. R. *Research Methodology*, 2nd Ed. Wiley Eastern, New Delhi (1985).

2. Kumar, R. *Research Methodology-A step by step guide for beginners*, 2nd Ed. PearsonEducation (2005).

2. Best, J. W.; Kahn, V. *Research in Education*, 8th Ed. PHI Publication (1998).

3. Krishnaswami, K. N. and others, *Management Research Methodology-Integration of principles,methods and Techniques*, 1st Ed. Pearson Education (2009).

LAB: (30 h)

Dissertation/Literature Survey/Seminar

CHE8104C: Inorganic Chemistry-V

Total lectures: 45(L+T) & 30 (P) Credits: 4 (Theory: 03, Lab: 01)

***Course objective:** Introduction to non-transition elements chemistry, including basic organometallic chemistry. Introductory ideas of solid states, and inorganic reaction mechanism and photochemistry*

Learning outcome: *Students will be able to apply their knowledge of inorganic and solid state chemistry in explaining, interpreting and critically examining bonding/structure/reactivity of metal complexes and organometallic compounds.*

Bonding in Inorganic and Coordination Compounds: (15h)

CFT and their limitations; ligand field theory, d-orbital wave functions, d-orbital splitting in octahedral, square planar, square pyramidal, trigonal bipyramidal, and tetrahedral complexes; Jahn-Teller distortion, CFSE for d^1 to d^{10} systems, pairing energy, low-spin and high-spin complexes, and molecular orbital (MO) theory of selected octahedral, tetrahedral complexes and other geometries, Walsh Diagram.

Electronic Spectra of Transition Metal Complexes: (10 h)

d-d transition, charge transfer transition, color, intensity and origin of spectra, interpretation, term symbols and splitting of terms different geometries, selection rules for electronic transitions, correlation, Tanabe-Sugano and Orgel diagrams, calculation of Dq, B and C, nephelauxetic ratio.

Magnetic Properties: (10 h)

Magnetic properties of free ions, types of magnetic behaviour: dia-, para-, ferro- and antiferro-magnetism, temperature independent paramagnetism, magnetic susceptibility - Van Vleck equation, experimental measurement, magnetic moment - orbital contribution, quenching of contribution, effect of spin orbit coupling, spincrossover. Temperature dependence of magnetic susceptibility, exchange coupling effects. Magnetic properties of second and third transition series and lanthanides.

Inorganic Photochemistry: (6 h)

Photosubstitution and photoredox reactions of chromium, cobalt and ruthenium compounds, Ligand field and charge transfer state (Thexi& DOSENCO states), cis-trans isomerization, photocatalysis and solar energy conversion by ruthenium complexes.

Molecular Symmetry and the Symmetry Groups: (10 h)

Symmetry elements and operations, classes of symmetry operations, symmetry point groups. Matrix notation for geometric transformations, reducible and irreducible representations, rules about irreducible representation as derived from great orthogonality theorem, relationship between reducible and irreducible groups, character tables.

Books Recommended:

1. J. E. Huheey, E. A. Keiter and R. L. Keiter; *Inorganic Chemistry: Principles of Structure and Reactivity*, 4th Ed. Pearson Education, 2006.

2. B. N. Figgis, M. A. Hitchman; *Ligand Field theory and its Applications*, Wiley India, 2010.

3. G. L. Miessler, D Tarr; *Inorganic Chemistry*. 3rd Ed., Pearson Education, 2004.

4. P. W. Atkins, T. Overton, J. Rourke, M. Weller, F. Armstrong; *Shriver &Atkins' Inorganic Chemistry*, 5th Ed. Oxford University Press, 2010.

5. *Fundamental Concepts of Inorganic Chemistry*, Vols. 1-7, by A.K. Das and M. Das, CBS Publishers and Distributors, 2015.

6. R. L. Dutta, A. Syamal, *Elements of Magnetochemistry*, 2nd Ed. Affiliated East-West Press Pvt. Ltd.- New Delhi, 2004.

7. F. E. Mabbs, D. J. Machin, *Magnetism and Transition Metal Complexes*, Dover Pub. Inc., 2008.

8. *Reaction Mechanism in Inorganic Chemistry* 2nd Ed. R. R. Jordan Oxford University Press, 1998.

9. F. Basolo, R. G. Pearson, *Mechanism of Inorganic Reactions* 2nd Ed. Wiley Eastern Pvt. Ltd. 1973.

10. D. M. Roundhill, *Photochemistry and Photophysics of Metal Complexes*; Plenum: New York, 1994.

11. *Photochemical Processes' in Volume 1*, Chapter 7.3 of *Comprehensive Coordination Chemistry*, G. Wilkinson (Editor-in-Chief), Pergamon Press, 1987.

12. H.J. Arnikar, *Essentials of Nuclear Chemistry*, 4th Ed. Wiley Eastern, New Delhi, 1995.

13. G. Friedlander, J.W. Kennedy, E. S. Macias, and J. M. Miller, *Nuclear & Radiochemistry*, 3rd Edition John Wiley, New York. 1981.

CHE8204C: Organic Chemistry-VI

Total lectures: 45(L+T) & 30 (P) Credits: 4 (Theory: 03, Lab: 01)

Course objective: *The objective of the course is to educate students on the various types of organic reactions, their mechanisms and applications.*
Learning outcome:*On the completion of the course students will acquire the detailed knowledge on photochemical, pericyclic, and Organic name reactions.*

Organic Photochemistry: (10h)

Introduction to organic photochemical-photophysical processes, chemiluminescence, photosensitization. Photochemistry of carbonyl compounds: α-cleavage, β-cleavage, intramolecular H-abstraction, addition to π-systems- Paterno-Buchi reaction; Photochemistry of olefins - photostereomutation of cis-trans isomers, optical pumping, cycloaddition, photochemistry of conjugated polyenes, photochemistry of vision, Photochemistry of enones; Photo-rearrangement reactions, di-π-methane rearrangement, Photo-rearrangement of cyclohexadienones, Barton rearrangement; Singlet oxygen photochemistry

Pericyclic Reactions: (20 h)

MO symmetry, FMO of conjugated polyenes. Woodward-Hoffmann principle of conservation of orbital symmetry, allowed and forbidden reactions, stereochemistry of pericyclic reactions, orbital symmetry correlation method, PMO method. Cycloaddition reactions: 2+2, 4+2 cycloadditions, 3+2 and 4+3 dipolar cycloadditions; stereoselectivity of the reactions, regioselectivity of 4+2 cycloaddition reaction.

Sigmatropic rearrangement: (m+n) sigmatropic rearrangement of hydrogen and chiral alkyl groups; Divinylcyclopropane rearrangement, fluxional molecules, stereoselectivity in Cope and Claisen rearrangement. Sommelet-Hauser rearrangement.

Electrocyclic reactions and cycloreversions: Conrotatory and disrotatory process, Stereoselectivity of the reactions.

Linear and nonlinear cheletropic rearrangement, theories of cheletropic reactions, stereoselectivity of the reactions.

Ene reactions: of 1,7-dienes, carbonyl enophiles, simple problems. Claisen rearrangement and its variants, aza-Cope rearrangement (Overman rearrangement), ene reaction (metallo-ene; Coniaene).

Retrosynthetic Analysis: (10 h)

Basic principles and terminology of retrosynthesis, synthesis of aromatic compounds, one group and two group C-X disconnections,

One group C-C and two group C-C disconnections, amine and alkene synthesis, important strategies of retrosynthesis, functional group transposition, important functional group interconversions

Protecting Groups: (5 h)

Protection and deprotection of hydroxy, carboxyl, carbonyl, carboxy amino groups and carbon-carbon multiple bonds; chemo- and regioselective protection and deprotection

Illustration of protection and deprotection in peptide and carbohydrate synthesis.

Recommended Books:

1. F. A. Cary, R. I. Sundberg, *Advanced Organic Chemistry*, Part A and B, 5th Edition, Springer, 2009.
2. M. B. Smith, *Organic Synthesis*, 2nd Edition, 2005
3. W. Carruthers and I. Coldham, *Modern Methods of Organic Synthesis*, First South Asian Edition 2005, Cambridge University Press.
4. J. Clayden, N. Greeves, S. Warren, *Organic Chemistry*, 2nd edition, OUP 2012
5. E. V. Anslyn, D. A. Dougherty, *Modern Physical Organic Chemistry*, University Science Books, 2005

LAB: (30 h)

Synthesis (2-Steps):

1. (Benzoin – Benzil – Benzilic acid) : Base catalysed, rearrangement

2. (Benzophenone – Benzopinacol – benzopinacolone) : Photochemical, rearrangement

3. (2-Hydroxyacetophenone – 1,3-diketone – Chromone) : Acid catalysed cyclisation

4. Solvent free reductive amination: Synthesis of imine from aldehyde and amine in solvent free condition and its reduction to amine using $NaBH_4$.

5. Oxidation of phenanthrene to phenanthrene-dione and its subsequent condensation to imidazophenanthrene derivative.

6. Multicomponent reaction of aldehyde, β-keto ester and urea/thiourea for the synthesis of dihydro-pyrimidine derivatives (Biginelli reaction)

7. Multicomponent reaction of aldehyde, β-keto ester and ammonia for the synthesis of dihydro-pyridine derivatives (Hantzsch Pyridine Synthesis)

Recommended Books:

1. B. S. Furniss, A. J. Hannaford, P. W. G. Smith, *Vogel's Textbook of Practical Organic Chemistry*, Pearson, 2012.
2. V. K. Ahluwalia, S. Dhingra, *Comprehensive Practical Organic Chemistry*, University Press.
3. F. G. Mann, B. C. Saunders, *Practical Organic Chemistry*, 3rd Edition Longman, 1978
4. Selected articles from *Journal of Chemical Education*, ACS Publications.

CHE8304C: Physical Chemistry-V

Total lectures: 45(L+T) & 30 (P) Credits: 4 (Theory: 03, Lab: 01)

Course objective: *Students will be introduced to the concepts of chemical kinetics, electrochemistry, molecular dynamics and fast reaction kinetics.*
Learning outcome: *Students will able to describe/examine the concepts and theories of chemical kinetics and electrochemistry, and the applications of molecular dynamics, fast reactions and energy storage.*

Advanced Chemical Kinetics: (8 h)

Steady state approximation and its applications, Oscillating reactions, chemical Chaos, Belousov-Zhabotinski reaction, straight-chain reaction-hydrogen halogen reactions, alkane pyrolysis, Branching-chain reactions- the hydrogen-oxygen reaction, explosion limits, Enzyme catalyzed reactions, Michaelis-Menten mechanism- Lineweaver-Burk and Eadie plots, enzymeinhibiton.

Molecular Reaction Dynamics: (9 h)

Collisions of real molecules- trajectory calculations, Laser techniques, reactions in molecular beam, - reaction dynamics, Estimation of activation energy and calculation of potential energy surface- the transition state theory (TST) of bimolecular gaseous reactions, statistical and thermodynamic

formulations. Comparison between TST and hard sphere collision theory, Theory of unimolecular reactions- Lindemann theory and its limitations, kinetics of reactions in solution-diffusion controlled and chemically controlled reactions, TST of reactions in solution- Bronsted and Bjerrum equation, effect of ionic strength, kinetic salt effect.

Study of Fast Reactions: (8 h)

Stopped flow technique, temperature and pressure jump methods, NMR studies in fast reactions, shock tube kinetics, relaxation kinetics, Linearized rate equation, relaxation time in single step fast reactions, determination of relaxation time.

Theories of Unimolecular Reactions: (6 h)

Drawbacks of Lindemann theory-Hinselwood modification, RRK theory, slaters treatment, RRKM theory.

Dynamic Electrochemistry: (8 h)

Ion-solvent interaction- the Born model, Thermodynamic parameters of ion solvent interactions-structural treatment, the ion-dipole model-its modifications, ion-quadrupole and ion-induced dipole interactions, Primary solution- determination of hydration number, compressibility method and viscosity-mobility method, Debye-Huckel theory of ion-ion interactions-derivation, validity and limitations, extended Debye-Huckel-Onsager equation. The random walk model of ionic diffusion-Einstein Smoluchowski reaction.

Theories of Electrical Interface: (6 h)

Electrocapillary phenomena- Lippmann equation, electron transfer at interfaces, polarizable and non-polarizable and nonpolarisable interfaces, Butler-Volmer equation, Tafel plot

Recommended Books:

1. P. Atkins and J. Paula, *Physical Chemistry*, 9th Edition, Oxford University Press, Oxford 2010.
2. I. R. Levine, *Physical Chemistry*, 6th Edition, McGraw Hill Education, 2011.
3. K. J. Laidler, *Chemical Kinetics*,3rd Edition, Pearson, 2012.
4. J. O. Bockris, A. K. N. Reddy, *Modern Electrochemistry Part 1, 2A and 2B*, 2nd Edition, Springer
5. A. J. Bard, L. R. Faulkner, *Electrochemical Methods Fundamentals and Applications*, 2nd edition, Willy India, 2006.

LAB: (30 h)

Kinetics by spectrophotometry, polarimetry and conductometry, Relative strength of two acids by conductance, Determination of a weak acid and a strong acid in mixture by potentiometry, Study of liquid-liquid phase diagram, Determination of fluoride by ion selective electrode, nitrate spectrophotometry, Determination of average molecular weight of a polymer by viscometry.

Study of excess adiabatic compressibility of binary system by ultrasonic interferometry, Simultaneous determination of CMC and partition equilibrium constant by spectroscopic method, Kinetics of the

catalytic decomposition of H_2O_2 by manganese (IV) oxide, Determination of CMC by Du NouyTensiometry, Micellar catalysis by spectroscopy, Determination of *pKa* by spectroscopy, Determination of stoichiometry and the stability constant of the complex formation, Determination of activation energy of reaction by polarimetry

Recommended Books:

1. Viswanathan, B., Raghavan, P. S. *Practical Physical Chemistry*, (Viva Books Pvt. Ltd., 2005).
2. James, A. M., Prichard, F. E. *Practical Physical Chemistry*, 3rd Edn., (Longman, 1974).
3. Jadav, J. B. *Advanced Practical Physical Chemistry*, (Krishna Prakashan, 2015).
4. Khosla, B. D.; Garg, V. C. & Gulati, A. *Senior Practical Physical Chemistry,* R. Chand & Co.: New Delhi (2011).
5. Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. *Experiments in Physical Chemistry 8th Ed.*; McGraw-Hill: New York (2003).

CHE8404C: Spectroscopy-II

Total lectures: 45(L+T) & 30 (P) Credits: 4 (Theory: 03, Lab: 01)

Course Objective: *Core course on spectroscopy, aimed at introducing students to the fundamental principles of NMR, ESR, Mössbauer spectroscopy and Mass spectrometry, with emphasis on application. Mössbauer spectroscopy will be dealt on an introductory level with selected examples.*
Learning outcome: *Students will be able to explain the basic working principle of magnetic resonance and mass spectroscopic techniques and their application in chemistry analysis.*

NMR Spectroscopy: (22h)

NMR phenomenon, Zeeman splitting, factors affecting sensitivity and resolution of a NMR spectrum, chemical shift tensor, ^{1}H NMR-inductive and anisotropic effects on chemical shifts (δ), chemical and magnetic equivalence.

Pulse and Fourier transformation in NMR. Introduction to 2D NMR (COSY, HSQC). T1, T2 and NOE.

Dynamic processes by VT NMR- restricted rotation (DMF, annulenes and related systems), ring inversion(cyclohexane), degenerate rearrangement (bullvalene) and fluxional inorganic molecules, fluxionality in organolithium compounds in solution.

NQR spectroscopy: Principles and applications.

NMR of Si, F, B and P nuclei. NMR of paramagnetic metal complexes-contact and pseudo-contact shifts; magnetic moment measurement. Introduction to solid-state NMR–CP MAS.

ESR Spectroscopy: (10 h)

ESR spectra of organic and inorganic compounds, ZFS, Kramer‘s degeneracy, determination of electronic structure, Zeeman splitting, g-values, hyperfine and super hyperfine coupling constants, practical considerations of measurements, and instrumentation

Mass Spectrometry: **(8h)**

Mass spectrometry: basic principles, ionization techniques, isotope abundance, molecular ion, fragmentation processes of organic molecules, deduction of structure through mass spectral fragmentation. ESI-MS and MALDI-MS-applications in biomolecules. Studies of inorganic/coordination and organometallic representative compounds. Instrumentation

Mössbauer Spectroscopy: (**5h)**

Principles, instrumentation and applications

Recommended Books:

1. C.N. Banwell, E. M. McCash, *Fundamentals of Molecular Spectroscopy*, 4th Edition, Tata McGraw Hill, 1994.
2. D.L. Pavia, G. M. Lampman, G. S. Kriz, *Introduction to Spectroscopy*, 4thEd. Brooks/Cole Cengage Learning, 2015.
3. R.S. Drago, *Physical Methods in Chemistry*, Saunders, Thomson Learning, 1977.
4. R.M Silverstein, F. X. Webster, D. J. Kiemle, D. L. Bryce, *Spectrometric Identifications of Organic Compounds*, 8th Edition, Wiley India Pvt. Ltd, 2015.
5. W. Kemp, *Organic Spectroscopy*, 3rd Edition, Palgrave Macmillan, 2011.
6. L. D. Field, S. Sternhell, J. R. Kalman, *Organic Structures from Spectra*, 5th Edition, John Wiley & Sons 2013
7. D.W.H. Rankin, N. Mitzel, C. Morrison, *Structural Methods in Molecular Inorganic Chemistry*, Wiley, 2013.

LAB: **(30 h)**

1. Quantitative determination of metal ions in given solution by spectroscopic methods
2. Spectroscopic methods for estimation of functional groups.
3. Estimating the formation/stoichiometry of donor-acceptor complex involving anthracene and picric acid (Job's method).
4. Determination of quantum yield of a chromophore/dye in a particular solvent.
5. Chiral resolution of a racemic mixture by crystallisation and determination of enantiomeric excess.

Recommended Books:

1. B. S. Furniss, A. J. Hannaford, P. W. G. Smith, *Vogel's Textbook of Practical Organic Chemistry*, Pearson, 2012.
2. V. K. Ahluwalia, S. Dhingra, *Comprehensive Practical Organic Chemistry*, University Press.
3. F. G. Mann, B. C. Saunders, *Practical Organic Chemistry*, 3rd Edition Longman, 1978
4. Selected articles from *Journal of Chemical Education*, ACS Publications.

Skill Enhancement Course

CHE1103SE: Fuel Chemistry

Total lectures: 45(L+T) Credits: 3 (Theory: 03, Lab: 00)

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

Learning Outcomes: *At the end of this course students will learn about the classes of renewable and non-renewable energy sources. Students will learn about the composition of coal and crude petroleum, their classification, isolation of coal and petroleum products and their usage in various industries. They will also learn to determine industrially significant physical parameters for fuels and lubricants.*

Introduction: (5 h)

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

Coal: (15 h)

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

Petroleum and Petrochemical Industry: (15 h)

Composition of crude petroleum, Refining and different types of petroleum products and their applications.

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

Lubricants: (10 h)

Classification of lubricants, lubricating oils (conducting and non-conducting)
Solid and semisolid lubricants, synthetic lubricants.
Properties of lubricants (viscosity index, cloud point, pore point) and their determination

Recommended Books:

1. E. Stocchi: *Industrial Chemistry*, Vol -I, Ellis Horwood Ltd. UK.

2. P.C. Jain, M. Jain: *Engineering Chemistry*, Dhanpat Rai & Sons, Delhi.
3. B.K. Sharma: *Industrial Chemistry,* Goel Publishing House, Meerut

CHE2103SE: Green Methods in Chemistry

Total lectures: 45(L+T) Credits: 3 (Theory: 03, Lab: 00)

Course Objectives: *This course introduces students to the utilization of green chemistry from industrial perspective and provides exposure to methods by which environmental problems are evaluated and designing of sustainable solutions.*
Learning Outcome: *Students shall be able to describe and evaluate chemical products and processes from environmental perspective, define and propose sustainable solutions and critically assess the methods for waste reduction and recycling.*

Introduction to Green Chemistry: (15 h)
Tools of Green chemistry, twelve principles of Green Chemistry, with examples.

The following Real-World Cases in Green Chemistry Should be Discussed: (30 h)
1. A green synthesis of ibuprofen which creates less waste and fewer byproducts (Atom economy).
2. Surfactants for Carbon Dioxide – replacing smog producing and ozone depleting solvents with CO_2 for precision cleaning and dry cleaning of garments.
3. Environmentally safe antifoulant.
4. CO_2 as an environmentally friendly blowing agent for the polystyrene foam sheet packaging market.
5. Using a catalyst to improve the delignifying (bleaching) activity of hydrogen peroxide.
6. A new generation of environmentally advanced preservative: getting the chromium and arsenic out of pressure treated wood.
7. Right fit pigment: synthetic azopigments to replace toxic organic and inorganic pigments.
8. Development of a fully recyclable carpet: cradle to cradle carpeting.

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

CHE3103SE: Basic Analytical Chemistry

Total lectures: 45(L+T) Credits: 3 (Theory: 03, Lab: 00)

Course Objective: *To familiarize students with different micro and semi micro analytical techniques and help develop the ability to use modern instrumental methods for chemical analysis of food, soil, air and water.*
Learning Outcome: *Upon completion of this course, students shall be able to explain the basic principles of chemical analysis, design/implement microscale and semi micro experiments, record, interpret and analyze data following scientific methodology.*

Introduction: (5 h)

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

Analysis of Soil: **(5 h)**

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

a. Determination of pH of soil samples.

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

Analysis of Water: **(5 h)**

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

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

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

Analysis of Food Products: **(8 h)**

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

a. Identification of adulterants in some common food items like coffee powder, asafoetida, chilli powder, turmeric powder, coriander powder and pulses, etc.

b. Analysis of preservatives and colouring matter.

Chromatography: **(5 h)**

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

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

b. To compare paint samples by TLC method.

Ion-exchange: **(4 h)**

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

Analysis of cosmetics: **(5 h)**

Major and minor constituents and their function

a. Analysis of deodorants and antiperspirants, Al, Zn, boric acid, chloride, sulphate.

b. Determination of constituents of talcum powder: Magnesium oxide, Calcium oxide, Zinc oxide and Calcium carbonate by complexometric titration.

Suggested Applications (Any one): **(2 h)**

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

b. To analyze arson accelerants.

c. To carry out analysis of gasoline.

Suggested Instrumental demonstrations: **(6 h)**

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

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

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

Recommended Books:

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

Interdisciplinary Course

CHE1103ID: History of Chemistry

Total lectures: 45(L+T) Credits: 3 (Theory: 03, Lab: 00)

Course Objective: *This course introduces students with historical development of chemistry.*

Learning Outcome: *On completion of this course, the students will be able to learn understanding of chemical science during different eras indifferent parts of the world, analyze the role played by the Chemical science in different eras in the evolution of modern-day science, and ethics in science*

Unit 1: (15 h)

Old traditions of Chemical sciences in various countries, Ancient Technology, Medicine in the ancient times, Ayurvedic Chemistry, Alchemy

India, Islamic & Chinese Alchemy, Metal extraction in the ancient times, Fiber, cloth and dying chemistry in the ancient times, Paper and ink in ancient times

Unit 2: (10 h)

Construction materials in the ancient times, The iron pillar of Delhi, Science & Technology in the West, Medieval and Renaissance Medicine

Unit 3: (10 h)

Modern traditions and methods, The Chemical Revolution: From Boyle to Dalton, Priestley's discovery of dephlogisticated air, Lavoisier and oxygen

Unit 4: (10 h)

Discoveries and Inventions in the context of state of art and impact, Development of chemistry during the industrial revolution, Development of chemistry during World War, Ethics in science.

Recommended Books:

1. Brock, W. H. *The Chemical Tree: A History of Chemistry*, W. W. (Norton & Co.: New York, 2000).

2. Bell, M. S. *Lavoisier in the Year One*, (W. W. Norton & Co.: New York, 2005).

3. Tripathi, V. Ed. *Archaeometallurgy in India*, (Cambridge University Press, 1998).

CHE2103ID: Environmental Chemistry

Total lectures: 45(L+T) Credits: 3 (Theory: 03, Lab: 00)

Course Objectives: *This course provides an introduction to the air, water & soil pollution and their effects on living organisms and the environment has also been covered. Students are also expected to learn about different kinds of wastes, their safe disposal and the importance of practicing green chemistry in chemical industry.*

Learning Outcomes: *After successful completion of the course, Students will learn about environmental pollution by various gaseous, liquid wastes and nuclear wastes and their effects on living beings. Finally, the students will learn about industrial waste management, their safe disposal and the importance of environment friendly "green chemistry" in chemical industry.*

Air Pollution: (15 h)

Ecosystems. Biogeochemical cycles of carbon, nitrogen and sulfur.
Major regions of atmosphere. Chemical and photochemical reactions in atmosphere. Air pollutants: types, sources, particle size and chemical nature; Photochemical
smog: its constituents and photochemistry. Environmental effects of ozone, Major sources of air pollution. Pollution by SO_2, CO_2, CO, NO_x, H_2S and other foul smelling gases. Methods of estimation of CO, NO_x, SO_x and control procedures. Effects of air pollution on living organisms and vegetation. Greenhouse effect and Global warming, Ozone depletion by oxides of nitrogen, chlorofluorocarbons and Halogens, removal of sulfur from coal. Control of particulates.

Water Pollution: (12 h)

Hydrological cycle, water resources, aquatic ecosystems, Sources and nature of water pollutants, Techniques for measuring water pollution, Impacts of water pollution on hydrological and ecosystems. Water purification methods. Effluent treatment plants (primary, secondary and tertiary treatment). Industrial effluents from the following industries and their treatment: electroplating, textile, tannery, dairy, petroleum and petrochemicals, agro, fertilizer, etc. Sludge disposal Industrial waste management, incineration of waste. Water treatment and purification (reverse osmosis, electro dialysis, ion exchange). Water quality parameters for waste water, industrial water and domestic water.

Soil Pollution: (12 h)

General types of soil colloids, the structure and properties of layer aluminosilicates, including types of charge, the phenomena and basis of ion exchange, soil-specific capacities for cation and anion exchange (CEC and AEC), and importance of these chemical reactions.
Definition of pH, its importance, sources of H^+ and OH^-, pH buffering in soils, and how it is managed with base (e.g., lime) or acid (e.g., sulphur) amendments.

Energy & Environment: (6 h)

Sources of energy: Coal, petrol and natural gas. Nuclear Fusion / Fission, Solar energy, Hydrogen, geothermal, Tidal and Hydel etc. Nuclear Pollution: Disposal of nuclear waste, nuclear disaster and its management.

Recommended Books:

1. K. De, *Environmental Chemistry*: New Age International Pvt., Ltd, New Delhi.
2. S. M. Khopkar, *Environmental Pollution Analysis*: Wiley Eastern Ltd, New Delhi.
3. S.E. Manahan, *Environmental Chemistry*, CRC Press (2005).
4. G.T. Miller, *Environmental Science* 11th edition. Brooks/ Cole (2006).
5. A. Mishra, *Environmental Studies*. Selective and Scientific Books, New Delhi (2005).

CHE3103ID: Chemistry in Humane Service

Total lectures: 45(L+T) Credits: 3 (Theory: 03, Lab: 00)

Course Objective: *This introductory chemistry course for non-science majors explores the intersection of chemistry with everyday life.*

Learning Outcome: *This course is intended for non-science students to develop an appreciation for the importance of the role of chemistry in everyday life, improve their ability to think critically and logical, make students more aware of the chemicals found in all aspects of daily life, become knowledgeable about the connection between chemistry and pollution, health care, nutrition and life. Furthermore, students will apply knowledge of chemistry to improve quality of life.*

Dairy Products: (7 h)

Composition of milk and milk products. Analysis of fat content, minerals in milk and butter. Estimation of added water in milk.

Food Additives, Adulterants and Contaminants: (15 h)

Food preservatives like benzoates, propionates, sorbates, disulphites. Artificial sweeteners: Aspartame, saccharin, dulcin, sucralose and sodium cyclamate.

Flavours: Vanillin, alkyl esters (fruit flavours) and monosodium glutamate.

Artificial food colorants: Coal tar dyes and non-permitted colours and metallic salts. Analysis of pesticide residues in food.

Beverage: Analysis of caffeine in coffee and tea, detection of chicory in coffee, chloral hydrate in toddy, estimation of methyl alcohol in alcoholic beverages.

Pharmaceuticals: (8 h)

Introduction, Contribution of chemistry to human health and historical developments in medicine, Classification of drugs and some common drugs used in our daily life.

Paints & Pigments: (15 h)

White pigments (white lead, ZnO, lithopone, TiO_2). Blue, red, yellow and green pigments. Paints and distempers: Requirement of a good paint. Emulsion, latex; luminescent paints. Fire retardant paints and enamels, lacquers. Solvents and thinners for paints.

Dyes: Colour and constitution (electronic concept). Classification of dyes. Methods of applying dyes to the fabrics. A general study of azo dyes, Mordant brown, Congo red and methyl orange.

Recommended Books:

1. B. K. Sharma: *Introduction to Industrial Chemistry*, Goel Publishing, Meerut (1998)
2. Analysis of Foods – H.E. Cox: 13. *Chemical Analysis of Foods* – H.E.Cox and Pearson.
3. *Foods: Facts and Principles*. N. Shakuntala Many and S. Swamy, 4th ed. New Age International (1998)

MINOR COURSES/PAPERS

CHE1104M: Chemistry-I

Total lectures: 45(L+T) & 30 (P) Credits: 4 (Theory: 03, Lab: 01)

Course Objective: *This course may be divided into three broad areas of chemistry- physical, organic and inorganic chemistry. In this course students will be taught basics of organic chemistry, atomic structure, gaseous and liquid state.*

Learning Outcome: *After completion of this course the students will learn the atomic structure through the basic concepts of quantum mechanics. They will learn about the states of matter, especially gaseous and liquid states. In organic part, the students are expected to learn basic ideas used in organic chemistry.*

Gaseous State: (**10 h**)

Kinetic molecular model of a gas: postulates and derivation of the kinetic gas equation; collision frequency; collision diameter; mean free path and viscosity of gases, including their temperature and pressure dependence, relation between mean free path and coefficient of viscosity, calculation of σ from η; variation of viscosity with temperature and pressure.

Maxwell distribution and its use in evaluating molecular velocities (average, root mean square and most probable) and average kinetic energy.

Behaviour of real gases: Deviations from ideal gas behaviour, compressibility factor, Z, and its variation with pressure for different gases. Causes of deviation from ideal behaviour. Vander Waals equation of state, its derivation and application in explaining real gas behaviour, Boyle temperature. critical state, relation between critical constants and van der Waals constants, law of corresponding states.

Liquid State: (**5 h)**

Physical properties of liquids; vapour pressure, surface tension and coefficient of viscosity, and their determination. Effect of addition of various solutes on surface tension and viscosity. Temperature variation of viscosity of liquids and comparison with that of gases.

Basics of Organic Chemistry: (15 h)

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

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

Homolytic and Heterolytic fission with suitable examples. Curly arrow rules, formal charges; Electrophiles and Nucleophiles; Nucleophlicity and basicity; Types, shape and their relative stability of Carbocations, Carbanions, Free radicals and Carbenes.

Introduction to types of organic reactions and their mechanism: Addition, Elimination and Substitution reactions.

Aromaticity: Hückel's rule, aromatic character of arenes, cyclic carbocations/carbanions and heterocyclic compounds with suitable examples.

Atomic Structure: (15 h)

Bohr's theory, its limitations and atomic spectrum of hydrogen atom. Wave mechanics: de Broglie equation, Heisenberg's Uncertainty Principle and its significance, Schrödinger's wave equation, significance of ψ and ψ^2. Quantum numbers and their significance. Normalized and orthogonal wave functions. Sign of wave functions. Radial and angular wave functions for hydrogen atom. Radial and angular distribution curves. Shapes of *s, p, d* and *f* orbitals. Contour boundary and probability diagrams. Pauli's Exclusion Principle, Hund's rule of maximum multiplicity, Aufbau's principle and its limitations, Variation of orbital energy with atomic number.

Recommended Books:

1.Lee, J. D. *Concise Inorganic Chemistry*, 5th Ed., Oxford University Press, 2008.
2. Douglas, B.E. and Mc Daniel, D.H., *Concepts and Models of Inorganic Chemistry*, 3rd Ed. Wiley India, 2006.
3. Morrison, R. N. & Boyd, R. N. *Organic Chemistry*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
4. Finar, I. L. *Organic Chemistry (Volume 1)*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
5. Peter, A. & Paula, J. de. *Physical Chemistry 9th Ed*., Oxford University Press (2011).
6. Castellan, G. W. *Physical Chemistry* 4th Ed., Narosa (2004).
7. Advanced Organic Chemistry; Reactions, Mechanisms and Structure; Jerry March

LAB: (30 h)

(i) Detection N, S, halogens in organic compounds.
(ii) Detection of Functional groups present in organic samples.

(iii) Titrimetric Analysis
(a) Calibration and use of common laboratory apparatus
(b) Preparation of solutions of different Molarity/Normality of titrants

Recommended Books:

1. Mann, F.G. & Saunders, B.C. *Practical Organic Chemistry*, Pearson Education (2009)
2. Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. *Practical Organic Chemistry*, 5th Ed., Pearson (2012)
3. Ahluwalia, V.K. & Aggarwal, R. *Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis*, University Press (2000).
4. Khosla, B. D.; Garg, V. C. & Gulati, A., *Senior Practical Physical Chemistry*, R. Chand & Co.: New Delhi (2011).

CHE2104M: Chemistry-II

Total lectures: 45(L+T) & 30 (P) Credits: 4 (Theory: 03, Lab: 01)

Course Objective: *This course may be divided into three broad areas of chemistry- physical, organic and inorganic chemistry. In this course students will be taught solid state, ionic equilibria, stereochemistry and periodicity of elements.*

Learning Outcome: *After completion of this course the students will learn the fundamental concepts of solid state and ionic equilibria along with conductance. They will understand the periodic properties of elements. In organic part, the students are expected to learn basic ideas stereochemistry.*

Solid State: (4 h)

Nature of the solid state, law of constancy of interfacial angles, law of rational indices, Miller indices, X-ray diffraction, Bragg's law, a simple account of rotating crystal method and powder pattern method. Analysis of powder diffraction patterns of NaCl, CsCl and KCl. Defects in crystals. Liquid crystals (Introductory idea)

Ionic equilibria and Conductance: (11 h)

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

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

Solubility and solubility product of sparingly soluble salts – applications of solubility product principle. Qualitative treatment of acid – base titration curves (calculation of pH at various stages). Theory of acid–base indicators; selection of indicators and their limitations.

Multistage equilibria in polyelectrolyte systems; hydrolysis and hydrolysis constants.

Arrhenius theory of electrolytic dissociation. Conductivity, equivalent and molar conductivity and their variation with dilution for weak and strong electrolytes. Molar conductivity at infinite dilution. Kohlrausch law of independent migration of ions. Debye-Hückel-Onsager equation, Wien effect, Debye-Falkenhagen effect, Walden's rules.

Stereochemistry: **(15 h)**

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

Optical Isomerism: Optical Activity, Specific Rotation, Chirality/Asymmetry, Enantiomers,

Molecules with two or more chiral-centres, Distereoisomers, meso structures, Racemic mixture and resolution. Relative and absolute configuration: D/L and R/S designations.

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

Periodicity of Elements: **(15 h)**

Long form of periodic table. s, p, d, f block elements. Detailed discussion of the following properties of the elements, with reference to s & p-block:
(a) Effective nuclear charge, shielding or screening effect, Slater rules, variation of effective nuclear charge in periodic table.
(b) Atomic radii (van der Waals)
(c) Ionic and crystal radii.
(d) Covalent radii (octahedral and tetrahedral)
(e) Ionization enthalpy, Successive ionization enthalpies and factors affecting ionization energy. Applications of ionization enthalpy.
(f) Electron gain enthalpy, trends of electron gain enthalpy.
(g) Electronegativity, Pauling's/Mulliken's/Allred Rachow's/ and Mulliken-Jaffé's electronegativity scales. Variation of electronegativity with bond order, partial charge, hybridization, group electronegativity. Sanderson's electron density ratio.

Recommended Books

1.Lee, J. D. *Concise Inorganic Chemistry*, 5th Ed., Oxford University Press, 2008.
2. Douglas, B.E. and Mc Daniel, D.H., *Concepts and Models of Inorganic Chemistry*, 3rd Ed. Wiley India, 2006.
3. Morrison, R. N. & Boyd, R. N. *Organic Chemistry*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
4. Finar, I. L. *Organic Chemistry (Volume 1)*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
5. Peter, A. & Paula, J. de. *Physical Chemistry* 9th Ed., Oxford University Press (2011).
6. Castellan, G. W. *Physical Chemistry* 4th Ed., Narosa (2004).

LAB: **(30 h)**

Acid-Base Titrations
(i) Estimation of carbonate and hydroxide present together in mixture.
(ii) Estimation of carbonate and bicarbonate present together in a mixture.
(iii) Estimation of free alkali present in different soaps/detergents
Oxidation-Reduction Titrimetry
(i) Estimation of Fe(II) and oxalic acid using standardized $KMnO_4$solution.
(ii) Estimation of oxalic acid and sodium oxalate in a given mixture.
(ii) Estimation of Fe(II) with $K_2Cr_2O_7$using internal (diphenylamine, anthranilic acid) and external indicator

Recommended Books:

1. Mann, F.G. & Saunders, B.C. *Practical Organic Chemistry*, Pearson Education (2009)
2. Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. *Practical Organic Chemistry*, 5th Ed., Pearson (2012)
3. Ahluwalia, V.K. & Aggarwal, R. *Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis*, University Press (2000).
4. Khosla, B. D.; Garg, V. C. & Gulati, A., *Senior Practical Physical Chemistry*, R. Chand & Co.: New Delhi (2011).
5. Mendham, J. et al.: *Vogel's Text Book of Quantitative Chemical Analysis*; 6th Ed. Pearson Education, 2009.

CHE3104M: Chemistry-III

Total lectures: 45(L+T) & 30 (P) Credits: 4 (Theory: 03, Lab: 01)

Course Objective: *This course may be divided into one broad area of inorganic chemistry. In the course students will be taught chemical bonding, molecular structure along with acids and bases.*

Learning Outcome: *After completion of this course the students will learn the chemical bonding through VB and MO approaches. They will also understand the basic concepts of acids and bases and their applications.*

Chemical Bonding and Molecular Structure: (30 h)

Ionic Bonding: General characteristics of ionic bonding. Energy considerations in ionic bonding, lattice energy and solvation energy and their importance in the context of stability and solubility of ionic compounds. Statement of Born-Landé equation for calculation of lattice energy, Born-Haber cycle and its applications, polarizing power and polarizability.
Fajan's rules, ionic character in covalent compounds, bond moment, dipole moment and percentage ionic character.

Covalent bonding: VB Approach: Shapes of some inorganic molecules and ions on the basis of VSEPR and hybridization with suitable examples of linear, trigonal planar, square planar, tetrahedral, trigonal bipyramidal and octahedral arrangements.
Concept of resonance and resonating structures in various inorganic and organic compounds.MO Approach: Rules for the LCAO method, bonding and antibonding MOs and their characteristics for *s-s*, *s-p* and *p-p* combinations of atomic orbitals, nonbonding combination of orbitals, MO treatment of

homonuclear diatomic molecules of 1st and 2nd periods (including idea of *s-p* mixing) and heteronuclear diatomic molecules such as CO, NO and NO^+. Comparison of VB and MO approaches.

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

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

Acids and Bases: **(15 h)**

Brönsted-Lowry concept of acid-base reactions, solvated proton, relative strength of acids, types of acid-base reactions, levelling solvents, Lewis acid-base concept, Classification of Lewis acids, Hard and Soft Acids and Bases (HSAB), Application of HSAB principle

Recommended Books:

1. J. D. Lee: *A new Concise Inorganic Chemistry*, E L. B. S.
2. F. A. Cotton & G. Wilkinson: *Basic Inorganic Chemistry*, John Wiley.
3. Douglas, McDaniel and Alexader: *Concepts and Models in Inorganic Chemistry*, John Wiley.
4. James E. Huheey, *Ellen Keiter and Richard Keiter: Inorganic Chemistry: Principles of Structure and Reactivity*, Pearson Publication.

LAB: **(30 h)**

1. Estimation of sodium carbonate and sodium hydrogen carbonate present in a mixture.
2. Estimation of oxalic acid by titrating it with $KMnO_4$.
3. Estimation of water of crystallization in Mohr's salt by titrating with $KMnO_4$.
4. Estimation of Fe (II) ions by titrating it with $K_2Cr_2O_7$ using internal indicator.
5. Estimation of Cu (II) ions iodometrically using $Na_2S_2O_3$.

Recommended Books:

1. *Vogel's Qualitative Inorganic Analysis*, A.I. Vogel, Prentice Hall, 7th Edition.
2. *Vogel's Quantitative Chemical Analysis*, A.I. Vogel, Prentice Hall, 6th Edition.

CHE3204M: Physical Chemistry-I

Total lectures: 45(L+T) & 30 (P) Credits: 4 (Theory: 03, Lab: 01)

Course Objective: *In this course the chemical thermodynamics, chemical equilibrium, solutions and colligative properties will be taught to the students. Another unit of this course is systems of variable compositions.*

Learning Outcome: *In this course the students are expected to learn laws of thermodynamics, thermochemistry, thermodynamic functions, relations between thermodynamic properties, Gibbs Helmholtz equation, Maxwell relations etc. Moreover, the students are expected to learn partial molar quantities, chemical equilibrium, solutions and colligative properties. After completion of this course, the students will be able to understand the chemical systems from thermodynamic point of view.*

Chemical Thermodynamics-I: (12 h)

Intensive and extensive variables; state and path functions; isolated, closed and open systems; zeroth law of thermodynamics.
First law: Concept of heat, *q*, work, *w*, internal energy, *U*, and statement of first law; enthalpy, *H*, relation between heat capacities, calculations of *q*, *w*, *U* and *H* for reversible, irreversible and free expansion of gases (ideal and van der Waals) under isothermal and adiabatic conditions. Law of equipartition of energy, degrees of freedom and molecular basis of heat capacities.
Thermochemistry: Heats of reactions: standard states; enthalpy of formation of molecules and ions and enthalpy of combustion and its applications; calculation of bond energy, bond dissociation energy and resonance energy from thermochemical data, effect of temperature (Kirchhoff's equations) and pressure on enthalpy of reactions. Adiabatic flame temperature, explosion temperature.

Chemical Thermodynamics-II: (18 h)

Second Law: Concept of entropy; thermodynamic scale of temperature, statement of the second law of thermodynamics; molecular and statistical interpretation of entropy. Calculation of entropy change for reversible and irreversible processes.

Third Law: Statement of third law, concept of residual entropy, calculation of absolute entropy of molecules.

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

*Systems of Variable Composition***:** Partial molar quantities, dependence of thermodynamic parameters on composition; Gibbs-Duhem equation, chemical potential of ideal mixtures, change in thermodynamic functions in mixing of ideal gases.

Chemical Equilibrium: (8 h)

Criteria of thermodynamic equilibrium, degree of advancement of reaction, chemical equilibria in ideal gases, concept of fugacity. Thermodynamic derivation of relation between Gibbs free energy of reaction and reaction quotient. Coupling of exoergic and endoergic reactions. Equilibrium constants and their quantitative dependence on temperature, pressure and concentration. Free energy of mixing and spontaneity; thermodynamic derivation of relations between the various equilibrium constants K_p, K_c and K_x. *Le Chatelier* principle (quantitative treatment); equilibrium between ideal gases and a pure condensed phase.

Solution and Colligative Properties: (7h)

Dilute solutions; lowering of vapour pressure, Raoult's and Henry's Laws and their applications. Excess thermodynamic functions. Thermodynamic derivation using chemical potential to derive relations between the four colligative properties [(i) relative lowering of vapour pressure, (ii) elevation of boiling point, (iii) Depression of freezing point, (iv) osmotic pressure] and amount of solute. Applications in calculating molar masses of normal, dissociated and associated solutes in solution.

Recommended Books:

1. Peter, A. & Paula, J. de. *Physical Chemistry 9th Ed.*, Oxford University Press (2011).
2. Castellan, G. W. *Physical Chemistry 4th Ed.*, Narosa (2004).
3. Engel, T. & Reid, P. *Physical Chemistry 3rd Ed.*, Prentice-Hall (2012).
4. McQuarrie, D. A. & Simon, J. D. *Molecular Thermodynamics* Viva Books Pvt. Ltd.: New Delhi (2004).
5. Assael, M. J.; Goodwin, A. R. H.; Stamatoudis, M.; Wakeham, W. A. & Will, S. *Commonly Asked Questions in Thermodynamics*. CRC Press: NY (2011).
6. Levine, I. N. *Physical Chemistry* 6th Ed., Tata Mc Graw Hill (2010).
7. Metz, C.R. *2000 solved problems in chemistry*, Schaum Series (2006)
8. Puri, B. R.; Sharma, L. R.; Pathania, M. S. Principles of Physical Chemistry, Vishal Publishing Co.; 47th Ed. (2017)
9. Kapoor, K. L. A Textbook of Physical Chemistry (Volume 2) McGraw Hill Education; Sixth edition (2019)

LAB: (30h)

Thermochemistry

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

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

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

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

(e) Determination of basicity/proticity of a polyprotic acid by the thermochemical method in terms of the changes of temperatures observed in the graph of temperature versus time for different additions of a base. Also calculate the enthalpy of neutralization of the first step.

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

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

Recommended Books:

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

CHE4104M: Chemistry-IV

Total lectures: 45(L+T) & 30 (P) Credits: 4 (Theory: 03, Lab: 01)

Course Objective: *This course introduces students with aliphatic hydrocarbons and biomolecules.*
Learning Outcome: *After completion of this course the students will learn about various biological organic molecules, functional groups, alkanes, alkenes, alkynes etc.*

Aliphatic Hydrocarbons: (25 h)

Functional group approach for the following reactions (preparations & reactions) to be studied in context to their structure.
Alkanes: (Upto 5 Carbons). *Preparation:* Catalytic hydrogenation, Wurtz reaction, Kolbe's synthesis, from Grignard reagent. *Reactions:* Free radical Substitution: Halogenation.

Alkenes: (Upto 5 Carbons) *Preparation:* Elimination reactions: Dehydration of alkenes and dehydrohalogenation of alkyl halides (Saytzeff's rule); cis alkenes (Partial catalytic hydrogenation) and trans alkenes (Birch reduction). *Reactions:* cis-addition (alk. $KMnO_4$) and trans-addition (bromine), Addition of HX (Markownikoff's and anti-Markownikoff's addition), Hydration, Ozonolysis, oxymecuration-demercuration, Hydroboration-oxidation.

Alkynes: (Upto 5 Carbons) *Preparation:* Acetylene from CaC_2 and conversion into higher alkynes; by dehalogenation of tetra halides and dehydrohalogenation of vicinal-dihalides. *Reactions:* formation of metal acetylides, addition of bromine and alkaline $KMnO_4$, ozonolysis and oxidation with hot alk. $KMnO_4$.

Nucleic Acids , Amino Acids, Peptides and Proteins (20h)

Components of nucleic acids; Nucleosides and nucleotides; Synthesis and reactions of: Adenine, Guanine, Cytosine, Uracil and Thymine; Polynucleotides: DNA and RNA; Amino acids, peptides and their classification. α-Amino Acids - Synthesis, ionic properties and reactions. Zwitterions, pKa values, isoelectric point and electrophoresis; Study of peptides: determination of their primary structures-end group analysis, methods of peptide synthesis. Synthesis of peptides using N-protecting, C-protecting and C-activating groups -Solid-phase synthesis.

Recommended Books:

1. T. W. Graham Solomon: *Organic Chemistry, John Wiley and Sons*.

2. Peter Sykes: *A Guide Book to Mechanism in Organic Chemistry*, Orient Longman.
3. E. L. Eliel: *Stereochemistry of Carbon Compounds*, Tata McGraw Hill.
4. I. L. Finar: *Organic Chemistry* (Vol. I & II), E. L. B. S.
5. R. T. Morrison & R. N. Boyd: *Organic Chemistry*, Prentice Hall.
6. Arun Bahl and B. S. Bahl: *Advanced Organic Chemistry,* S. Chand

LAB: (30 h)

1. Detection of extra elements (N, S, Cl, Br, I) in organic compounds (containing upto two extra elements)
2. Separation of mixtures by Chromatography: Measure the R_f value in each case (combination of two compounds to be given)
(a) Identify and separate the components of a given mixture of 2 amino acids (glycine, aspartic acid, glutamic acid, tyrosine or any other amino acid) by paper chromatography
(b) Identify and separate the sugars present in the given mixture by paper chromatography.

Recommended Books:
1. *Textbook of Practical Organic Chemistry,* A.I. Vogel , Prentice Hall, 5th edition.
2. *Practical Organic Chemistry*, F. G. Mann. & B. C. Saunders, Orient Longman, 1960.

CHE4204M: ORGANIC CHEMISTRY-I

Total lectures: 45(L+T) & 30 (P) Credits: 4 (Theory: 03, Lab: 01)

Course Objective*: The course intrudes students to different classes of N-based compounds, including alkaloids and terpenoids and their potential application. Students are expected to learn about different classes of N-based compounds; their structures, synthesis and reactivity.*
Learning Outcome: *Students shall demonstrate the ability to identify and classify different types of N-based derivatives, alkaloids and heterocyclic compounds/explain their structure mechanism and reactivity/critically examine their synthesis and reactions mechanism.*

Carboxylic Acids and their Derivatives: (10 h)

Preparation, physical properties and reactions of monocarboxylic acids: Typical reactions of dicarboxylic acids, hydroxy acids and unsaturated acids: succinic/phthalic, lactic, malic, tartaric, citric, maleic and fumaric acids.

Preparation and reactions of acid chlorides, anhydrides, esters and amides; Comparative study of nucleophilic substitution at acyl group -Mechanism of acidic and alkaline hydrolysis of esters, Claisen condensation, Dieckmann and Reformatsky reactions, Hofmann bromamide degradation and Curtius rearrangement.

Sulphur and Nitrogen Containing Compounds: (15 h)

Preparation and reactions of thiols, thioethers and sulphonic acids.

Preparation and important reactions of nitro and compounds, nitriles and isonitriles.

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

Diazonium Salts: Preparation and their synthetic applications.

Heterocyclic Compounds: (10h)

Classification and nomenclature, Structure, aromaticity in 5-numbered and 6-membered rings containing one heteroatom;

Synthesis, reactions and mechanism of substitution reactions of: Furan, Pyrrole (Paal-Knorr synthesis, Knorr pyrrole synthesis, Hantzsch synthesis), Thiophene, Pyridine (Hantzsch synthesis), Pyrimidine. Indole: Fischer indole synthesis and Madelung synthesis).

Polynuclear Aromatic Hydrocarbons: (10h)

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

Recommended Books:

1. Morrison, R. T. & Boyd, R. N. *Organic Chemistry*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
2. Finar, I. L. *Organic Chemistry* (*Volume 1*), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
3. Graham Solomons, T.W. *Organic Chemistry*, John Wiley & Sons, Inc.
4. Clayden, J., Greeves, N. & Warren, S. *Organic Chemistry*, Second edition, Oxford University Press, 2012.
5. Keeler, J., Wothers, P. *Chemical Structure and Reactivity – An Integrated approach*, Oxford University Press.
6. Smith, J. G. *Organic Chemistry*, Tata McGraw-Hill Publishing Company Limited.
7. Carey, F. A.; Sundberg, R. J. *Advanced Organic Chemistry: Reactions and Synthesis (Part B)*, Springers.

LAB: (30 h)

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

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

a. Using conventional method.
b. Using green approach

ii. Benzolyation of one of the following amines (aniline, *o*-, *m*-, *p*- toluidines and *o*-, *m*-, *p*-anisidine) and one of the following phenols (β-naphthol, resorcinol, pcresol) by Schotten-Baumann reaction.
iii. Oxidation of ethanol/ isopropanol (Iodoform reaction).
iv. Bromination of any one of the following:
a. Acetanilide by conventional methods
b. Acetanilide using green approach (Bromate-bromide method)
v. Nitration of any one of the following:
a. Acetanilide/nitrobenzene by conventional method
b. Salicylic acid by green approach (using ceric ammonium nitrate). vi. Selective reduction of *meta* dinitrobenzene to *m*-nitroaniline.
vii. Reduction of *p*-nitrobenzaldehyde by sodium borohydride.
viii. Hydrolysis of amides and esters.
ix. Semicarbazone of any one of the following compounds: acetone, ethyl methyl ketone, cyclohexanone, benzaldehyde.
x. *S*-Benzylisothiouronium salt of one each of water soluble and water insoluble acids (benzoic acid, oxalic acid, phenyl acetic acid and phthalic acid).
xi. Aldol condensation using either conventional or green method.
xii. Benzil-Benzilic acid rearrangement.
The above preparations should be done using 0.5-1g of the organic compound. The solid samples must be collected and may be used for recrystallization, melting point and TLC.

Recommended Books:

1. Mann, F.G. & Saunders, B.C. *Practical Organic Chemistry*, Pearson Education (2009)
2. Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. *Practical Organic Chemistry, 5th Ed.*, Pearson (2012)
3. Ahluwalia, V.K. & Aggarwal, R. *Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis*, University Press (2000).
4. Ahluwalia, V.K. & Dhingra, S. *Comprehensive Practical Organic Chemistry: Qualitative Analysis*, University Press (2000).
5. Vogel, A. I. *Elementary Practical Organic Chemistry*, Part 1: *Small scale Preparations*, CBS Publishers and Distributors.

CHE5104M: Chemistry-V

Total lectures: 45(L+T) & 30 (P) Credits: 4 (Theory: 03, Lab: 01)

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

Learning Outcome: *After completion of this course the students will learn periodic properties in main group elements, transition metals (3d series). They will also learn the crystal field theory in coordination chemistry unit. In physical chemistry part, the students are expected to learn kinetic*

theory of gases, ideal gas and real gases, surface tension, viscosity, basic solid state chemistry and chemical kinetics.

s- and p-Block Elements: (15 h)

Periodicity in *s*- and *p*-block elements with respect to electronic configuration, atomic and ionic size, ionization enthalpy, electronegativity (Pauling, Mulliken, and Alfred-Rochowscales). Allotropy in C, S, and P.
Oxidation states with reference to elements in unusual and rare oxidation states like carbides and nitrides), inert pair effect, diagonal relationship and anomalous behaviour of first member of each group.

Transition Elements (3d series): (10 h)

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

Coordination Chemistry: (20 h)
Coordination compounds, types of ligands, Werner's theory, IUPAC nomenclature and isomerism in coordination compounds. Stereochemistry of complexes with 4 and 6 coordination numbers. Drawbacks of VBT. Crystal field effect, octahedral symmetry. Crystal field stabilization energy (CFSE), Crystal field effects for weak and strong fields. Tetrahedral symmetry. Factors affecting the magnitude of D. Spectrochemical series. Comparison of CFSE for O_h and T_d complexes, Tetragonal distortion of octahedral geometry. Jahn-Teller distortion, Square planar coordination.

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

LAB: (30h)

1.Semi-micro qualitative analysis using H2S of mixtures - not more than four ionic species (two anions and two cations and excluding insoluble salts) out of the following:
CO_3^{2-}, NO_2^-, S^{2-}, SO_3^{2-}, $S_2O_3^{2-}$, CH_3COO^-, F^-, Cl^-, Br^-, I^-, NO_3^-, BO_3^{3-}, $C_2O_4^{2-}$, PO_4^{3-}, NH_4^+, K^+, Pb^{2+}, Cu^{2+}, Cd^{2+}, Bi^{3+}, Sn^{2+}, Sb^{3+}, Fe^{3+}, Al^{3+},, Cr^{3+}, Zn^{2+}, Mn^{2+}, Co^{2+}, Ni^{2+}, Ba^{2+},Sr^{2+}, Ca^{2+}, Mg^{2+}
(Spot tests should be carried out wherever feasible)

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

3. Draw calibration curve (absorbance at λ_{max} vs. concentration) for various concentrations of a given coloured compound ($KMnO_4$/ $CuSO_4$) and estimate the concentration of the same in a given solution.

4. Determine the composition of the Fe^{3+}-salicylic acid complex solution by Job's method.

5. Estimation of (i) Mg^{2+} or (ii) Zn^{2+} by complexometric titrations using EDTA.
6. Estimation of total hardness of a given sample of water by complexometric titration.
7. Determination of concentration of Na^+ and K^+ using Flame Photometry.

Reference Books:

1. Svehla, G. *Vogel's Qualitative Inorganic Analysis*, Pearson Education, 2012.
2. Mendham, J. *Vogel's Quantitative Chemical Analysis*, Pearson, 2009.

CHE5204M: Inorganic Chemistry-I

Total lectures: 45(L+T) & 30 (P) Credits: 4 (Theory: 03, Lab: 01)

Course Objective: *This course introduces students to coordination chemistry. Various aspects like nomenclature, structure, bonding, variety and reactivity of the coordination compounds are included for the students to appreciate. Bioinorganic chemistry is included in this course to acquaint students on the useful and harmful aspects of metals in biological systems. Through the accompanying lab course, experiments related to gravimetric analysis, synthesis of coordination compounds and separation of metal ions using chromatography is included. This will broaden the experimental skills of the students where students will learn about various aspects of experiment design depending upon the requirements like synthesis, estimation or separation.*

Learning Outcome: *On successful completion, students will be able name coordination compounds according to IUPAC, explain bonding in this class of compounds, understand their various properties in terms of CFSE and predict reactivity. Students will be able to appreciate the general trends in the properties of transition elements in the periodic table and identify differences among the rows. Through the experiments students not only will be able to prepare, estimate or separate metal complexes/compounds but also will be able to design experiments independently which they should be able to apply if and when required.*

Coordination Chemistry: (20 h)

Coordination compounds, types of ligands, Werner's theory, IUPAC nomenclature and isomerism in coordination compounds. Stereochemistry of complexes with 4 and 6 coordination numbers. Valence bond theory (inner and outer orbital complexes), electroneutrality principle and back bonding. Crystal field theory, measurement of 10 Dq (Δ_o), CFSE in weak and strong fields, pairing energies, factors affecting the magnitude of 10 Dq (Δ_o, Δ_t).Octahedral vs. tetrahedral coordination, tetragonal distortions from octahedral geometry Jahn-Teller theorem, square planar geometry. Qualitative aspects of ligand field and MO Theory. Chelate effect, polynuclear complexes.

Transition Elements: (12 h)

General group trends with special reference to electronic configuration, colour, variable valency, magnetic and catalytic properties, ability to form complexes. Stability of various oxidation states and e.m.f. (Latimer & Frost diagrams). Difference between the first, second and third transition series.
Chemistry of Ti, V, Cr Mn, Fe and Co (Chemistry of first -row transition elements) in various oxidation states as halides, oxides, hydroxides.

Lanthanoids and Actinoids: (5 h)

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

Bioinorganic Chemistry: (8 h)

Metal ions present in biological systems, classification of elements according to their action in biological system. Geochemical effect on the distribution of metals. Sodium / K-pump, carbonic anhydrase and carboxypeptidase. Excess and deficiency of some trace metals. Toxicity of metal ions (Hg, Pb, Cd and As), reasons for toxicity, Use of chelating agents inmedicine.

Iron and its application in bio-systems, Haemoglobin, Storage and transfer of iron.

Recommended Books:

1. Cotton, F.A., Wilkinson, G. and Gaus, P. L., *Basic Inorganic Chemistry*, 3rd Ed., Wiley, 2007.

2. Huheey, J. E., Keiter, E. A., Keiter, R. L., Medhi, O. K., *Inorganic Chemistry: Principles of Structure and Reactivity*, 4th Ed., Pearson Education India, 2006.

3. Lippard, S.J. & Berg, J.M. *Principles of Bioinorganic Chemistry*, Panima Publishing Company, 1994.

4. Cotton, F.A. & Wilkinson, G, *Advanced Inorganic Chemistry*. 6th Ed., Wiley-VCH, 2007.

5. Basolo, F, and Pearson, R.C., *Mechanisms of Inorganic Chemistry*, John Wiley &Sons, NY, 1967.

6. Greenwood, N.N. &Earnshaw, A., *Chemistry of the Elements*, 2nd Ed., Elsevier India, 2010.

LAB: (30 h)

Gravimetric Analysis:

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

ii. Estimation of copper as CuSCN

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

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

Inorganic Preparations:

i. Tetraamminecopper(II) sulphate, $[Cu(NH_3)_4]SO_4.H_2O$

ii. Cis and trans $K[Cr(C_2O_4)_2.(H_2O)_2]$ Potassium dioxalatodiaquachromate (III)

iii. Tetraamminecarbonatocobalt (III) ion

iv. Potassium tris(oxalato)ferrate(III)

Chromatography of Metal Ions:

Principles involved in chromatographic separations. Paper chromatographic separation offollowing metal ions:

i. Ni(II) and Co(II)

ii. Fe(III) and Al(III)

Recommended Books:

1. Mendham, J. et al.: *Vogel's Textbook of Quantitative Chemical Analysis* ; 6th Ed. Pearson Education, 2009.

2. Marr, G. and Rockett, R.W. *Practical Inorganic Chemistry*, Van Nostrand Reinhold. 1972.

3. *Inorganic Syntheses*, Vol. 1-10.

CHE5304: Quantum Chemistry

Total lectures: 45(L+T) & 30 (P) Credits: 4 (Theory: 03, Lab: 01)

Course Objective: *The aim of this course is to introduce the students with two important areas- quantum chemistry and chemical bonding. In quantum chemistry unit the students will be taught the postulates of quantum mechanics and the application of quantum mechanical ideas in some simple systems such as particle in a box, rigid rotor, simple harmonic oscillator etc.*

Learning Outcome: *After completion of this course the students are expected to understand the foundation of quantum mechanics and its application in some simple chemical systems such as hydrogen atom or hydrogen like ions. The students will also learn chemical bonding in some simple molecular systems.*

Postulates of Quantum Mechanics: (6 h)

Postulates of quantum mechanics, quantum mechanical operators, Schrödinger equation.

Models in Quantum Chemistry: (14 h)

Free particle and "particle-in-a-box" (rigorous treatment), quantization of energy levels, zero-point energy Extension to two and three dimensional boxes, separation of variables, degeneracy. Qualitative treatment of simple harmonic oscillator model of vibrational motion: Setting up of Schrödinger equation and discussion of solution and wavefunctions. Vibrational energy of diatomic molecules and zero-point energy.

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

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

Structure of One-Electron Systems: **(5 h)**

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

Chemical Bonding: **(20 h)**

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

Covalent bonding, valence bond and molecular orbital approaches, LCAO-MO treatment of H_2^+. Bonding and antibonding orbitals. Qualitative extension to H_2. Comparison of LCAO-MO and VB treatments of H2 (only wavefunctions, detailed solution not required) and their limitations. Refinements of the two approaches (Configuration Interaction for MO, ionic terms in VB). Qualitative description of LCAO-MO treatment of homonuclear and heteronuclear diatomic molecules (HF, LiH). Localised and non-localised molecular orbitals treatment of triatomic (BeH_2, H_2O) molecules. Qualitative MO theory and its application to AH_2 type molecules.

Recommended Books:

1. McQuarrie, D. A. *Quantum Chemistry*, Viva Books (2016)
2. Chandra, A. K. *Introductory Quantum Chemistry* Tata McGraw-Hill (2001).
3. House, J. E. *Fundamentals of Quantum Chemistry 2nd Ed*. Elsevier: USA (2004).
4. Lowe, J. P. & Peterson, K. *Quantum Chemistry*, Academic Press (2005).
5. Sen, B. K. *Quantum Chemistry- Including Spectroscopy*, Kalyani Publishers; 4th edition (2011).
6. Kapoor, K. L. *A Textbook of Physical Chemistry (Volume 4)* McGraw Hill Education; 5th edition (2017).
7. Kakkar, R. *Atomic & Molecular Spectroscopy*, Cambridge University Press (2015).
8. Banwell, C. N. &McCash, E. M. *Fundamentals of Molecular Spectroscopy 4th Ed*. Tata McGraw-Hill: New Delhi (2006).

LAB: **(30 h)**

1. Introduction to open-source computational chemistry tools
2. Molecular modeling
3. Single-point energy calculation of chemical systems in their ground and excited electronic states
4. Geometry optimization of molecules
5. Energy calculations of conformers
6. Energy calculation of molecules in solvent system (discrete)

Recommended Books:

1.Lewars, E. *Computational Chemistry*, (Springer, 2003).

CHE6104M: Chemistry-VI

Total lectures: 45(L+T) & 30 (P) Credits: 4 (Theory: 03, Lab: 01)

Course Objective: *This course introduces three important topics of physical chemistry-solutions, phase equilibria and chemical kinetics.*
Learning Outcome: *After completion of this course the students will learn fundamental concepts behind solutions and phase of a system. Students are also expected to understand various concepts of chemical kinetics.*

Solutions: (15 h)

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

Phase Equilibrium: (15 h)

Phases, components and degrees of freedom of a system, criteria of phase equilibrium. Gibbs Phase Rule and its thermodynamic derivation. Derivation of Clausius – Clapeyron equation and its importance in phase equilibria. Phase diagrams of one-component systems (water and sulphur) and two component systems involving eutectics, congruent and incongruent melting points (lead-silver, FeCl3-H2O and Na-K only).

Chemical Kinetics: (15 h)

The concept of reaction rates. Effect of temperature, pressure, catalyst and other factors on reaction rates. Order and molecularity of a reaction. Derivation of integrated rate equations for zero, first and second order reactions (both for equal and unequal concentrations of reactants). Half–life of a reaction. General methods for determination of order of a reaction. Concept of activation energy and its calculation from Arrhenius equation. Theories of Reaction Rates: Collision theory and Activated Complex theory of bimolecular reactions. Comparison of the two theories (qualitative treatment only).

Reference Books:
1. Barrow, G.M. *Physical Chemistry* Tata McGraw-Hill (2007).
2. Castellan, G.W. *Physical Chemistry* 4th Ed. Narosa (2004).
3. Kotz, J.C., Treichel, P.M. & Townsend, J.R. *General Chemistry* Cengage LearningIndia Pvt. Ltd., New Delhi (2009).
4. Mahan, B.H. *University Chemistry* 3rd Ed. Narosa (1998).
5. Petrucci, R.H. *General Chemistry* 5th Ed. Macmillan Publishing Co.: New York (1985).

LAB: (30h)

Phase equilibria

a) Construction of the phase diagram of a binary system (simple eutectic) using cooling curves.

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

c) Study of the variation of mutual solubility temperature with concentration for the phenol-water system and determination of the critical solubility temperature.

Chemical Kinetics

Study the kinetics of the following reactions.

a) Initial rate method: Iodide-persulphate reaction

b) Integrated rate method:

c) Acid hydrolysis of methyl acetate with hydrochloric acid.

d) Saponification of ethyl acetate.

e) Compare the strengths of HCl and H_2SO_4 by studying kinetics of hydrolysis of methyl acetate

Reference Books:

1. Khosla, B. D.; Garg, V. C. & Gulati, A. *Senior Practical Physical Chemistry,* R. Chand & Co.: New Delhi (2011).

CHE6204M: Organic Chemistry-II

Total lectures: 45(L+T) & 30 (P) Credits: 4 (Theory: 03, Lab: 01)

Course Objectives*: This is a basic course in organic reagents and provides introduction to carbohydrate chemistry, dyes and polymers. Students are expected to learn about the different oxidizing and reducing agents and their applications in organic chemistry. Students shall be apprised with carbohydrate chemistry, dyes and polymers and their structure, reactivity and chemical properties.*

Learning Outcome*: Students will be able to explain/describe basic principles of different reagents and their importance in chemical/organic synthesis. Students shall be able to classify/identify/critically examine carbohydrates, polymers and dye materials.*

Oxidation Reactions: (10 h)

Metal based and non-metal based oxidations (Cr, Mn, Al, Ag, Os, Ru, Se, DMSO, hypervalent iodine and TEMPO based reagents). Reagents (Fremy‘s salt, silver carbonate, peroxides/per-acids). Sharpless asymmetric epoxidation, Jacobsen epoxidation, Shi epoxidation, Sharpless asymmetric dihydroxylation, Baeyer-Villiger oxidation, Wacker oxidation, hydroboration-oxidation, Prevost reaction and Woodward modification.

Reduction Reactions: (12 h)

Catalytic hydrogenation (Pd/Pt/Rh/Ni). Wilkinson catalyst, Noyori asymmetric hydrogenation, Metal based reductions using Li/Na/Ca in liquid ammonia, Sodium, Magnesium, Zinc, Titanium and Samarium (Birch, Pinacol formation, McMurry, Acyloin formation, dehalogenation and deoxygenations); Hydride transfer reagents from Group III and Group IV in reductions ($NaBH_4$ triacetoxyborohydride, L-selectride, K-selectride, Luche reduction, $LiAlH_4$, DIBAL-H, and Red-Al, Trialkylsilanes and Trialkylstannane, Meerwein-Pondorff-Verley reduction); Stereo/enantioselective reductions (Chiral Boranes, Corey-Bakshi-Shibata).

Carbohydrates: **(7h)**

Occurrence, classification and their biological importance.

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

Disaccharides – Structure elucidation of maltose, lactose and sucrose.

Polysaccharides – Elementary treatment of starch, cellulose and glycogen.

Dyes: **(6h)**

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

Alkaloids and Terpenes: **(10h)**

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

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

Recommended Books:

1. Banwell, C. N. &Mc.Cash, E. M. *Fundamentals of Molecular Spectroscopy*, 4th Edition, McGraw Hill.
2. Pavia, Lampman, Kriz& Vyvyan, *Introduction to Spectroscopy*, 5th Edition, CENGAGE Learing.
3. Silverstein, R. M.; Webster, F. X.; Kiemle, D. J. & Bryce, D. L. *Spectrometric Identification of Organic Compounds*, 8th Edition, Wiley.
4. Kemp, W. *Organic Spectroscopy*, Palgrave.
5. Kalsi, P. S. *Textbook of Organic Chemistry 1st Ed.*, New Age International (P) Ltd. Pub.
6. Morrison, R. T. & Boyd, R. N. *Organic Chemistry*, Dorling Kindersley (India)
Pvt. Ltd. (Pearson Education).
7. Billmeyer, F. W. *Textbook of Polymer Science*, John Wiley & Sons, Inc.
8. Gowariker, V. R.; Viswanathan, N. V. & Sreedhar, J. *Polymer Science*, New Age International (P) Ltd. Pub.
9. Finar, I. L. *Organic Chemistry* (*Volume 2: Stereochemistry and the Chemistry of Natural Products*), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
10. Graham Solomons, T.W. *Organic Chemistry*, John Wiley & Sons, Inc.
11. Clayden, J.; Greeves, N.; Warren, S.; Wothers, P.; *Organic Chemistry*, Oxford University Press.
12. Singh, J.; Ali, S.M. & Singh, J. *Natural Product Chemistry*, Prajati Prakashan (2010).

LAB: **(30 h)**

1. Extraction of caffeine from tea leaves.
2. Preparation of sodium polyacrylate.

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

Recommended Books:

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

CHE6304M: Spectroscopy

Total lectures: 45(L+T) & 30 (P) Credits: 4 (Theory: 03, Lab: 01)

Course Objective: *The aim of this course is to introduce the students with important areas of molecular spectroscopy and its application. In spectroscopy unit, rotational, vibrational, Raman, electronic, spin resonance, and electronic spectroscopy will be introduced.*
Learning Outcome: *After completion of this course the students are expected to understand the application of various kinds of spectroscopic techniques.*

Introduction to Molecular Spectroscopy: (5 h)

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

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

Vibrational Spectroscopy: (15 h)

Classical equation of vibration, computation of force constant, amplitude of diatomic molecular vibrations, anharmonicity, Morse potential, dissociation energies, fundamental frequencies, overtones, hot bands, degrees of freedom for polyatomic molecules, modes of vibration, concept of group frequencies. Vibration-rotation spectroscopy: diatomic vibrating rotator, P, Q, R branches. Fundamental and non-fundamental molecular vibrations; IR absorption positions of O, N and S containing functional groups; Effect of H-bonding, conjugation, resonance and ring size on IR absorptions; Fingerprint region and its significance; application in functional group analysis.

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

Electronic Spectroscopy: (15 h)

Franck-Condon principle, electronic transitions, singlet and triplet states, fluorescence and phosphorescence, dissociation and predissociation, calculation of electronic transitions of polyenes using free electron model. Types of electronic transitions, λ_{max}, Chromophores and Auxochromes, Bathochromic and Hypsochromic shifts, Intensity of absorption; Application of Woodward Rules for calculation of λ_{max} for the following systems: α,β-unsaturated aldehydes, ketones, carboxylic acids and esters; Conjugated dienes: alicyclic, homoannular and heteroannular; Extended conjugated systems (aldehydes, ketones and dienes); distinction between cis and trans isomers.

NMR and ESR Spectroscopy: (10 h)

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

Electron Spin Resonance spectroscopy: Its principle, hyperfine structure, ESR of simple radicals.

Applications of IR, UV and NMR for identification of simple organic and inorganic molecules.

Recommended Books:

1. Banwell, C. N. &McCash, E. M. *Fundamentals of Molecular Spectroscopy* 4th Ed. Tata McGraw-Hill: New Delhi (2006).
2. Kakkar, R. *Atomic & Molecular Spectroscopy*, Cambridge University Press (2015).
3. *Introduction to Spectroscopy* by D. L. Pavia; G. M. Lampman and G. S. Kriz

LAB: (30 h)

UV/Visible Spectroscopy

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

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

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

4. Verify Lambert-Beer's law and determine the concentration of

$CuSO_4$/$KMnO_4$/$K_2Cr_2O_7$in a solution of unknown concentration

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

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

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

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

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

10. Analysis of the given vibration-rotation spectrum of HCl(g)

Recommended Books:

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

CHE7104M: Chemistry-VII

Total lectures: 45(L+T) & 30 (P) Credits: 4 (Theory: 03, Lab: 01)

Course Objective: *In this course students will be taught chemical energetic, chemical equilibrium and electrochemistry.*
Learning Outcome: *After completion of this course the students will able to understand the chemical system from thermodynamic points of view. They will also learn two very important topics in chemistry- chemical equilibrium and electrochemistry.*

Chemical Energetics: (20 h)

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

Chemical Equilibrium: (10 h)

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

Electrochemistry: (15 h)

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

Recommended Books:

1. G. M. Barrow: *Physical Chemistry* Tata McGraw---Hill (2007).

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

LAB: (30h)

Thermochemistry
1. Determination of heat capacity of calorimeter for different volumes.
2. Determination of enthalpy of neutralization of hydrochloric acid with sodium hydroxide.
3. Determination of enthalpy of ionization of acetic acid.
4. Determination of integral enthalpy of solution of salts (KNO_3, NH_4Cl).
5. Determination of enthalpy of hydration of copper sulphate.
6. Study of the solubility of benzoic acid in water and determination of ΔH.

Potentiometry
Perform the following potentiometric titrations:
v. Strong acid vs. strong base
vi. Weak acid vs. strong base
vii. Potassium dichromate vs. Mohr's salt

Recommended Books
1. B.D. Khosla, *Senior Practical Physical Chemistry*, R. Chand & Co.

CHE7204M: Inorganic Chemistry-II

Total lectures: 45(L+T) & 30 (P) Credits: 4 (Theory: 03, Lab: 01)

Course Objective: *This is an introductory course on inorganic chemistry, through which students will appreciate the chemistry of the transition metals, aspects related to bonding, oxidation states and electronic/magnetic properties.*
Learning Outcome: *Students will be able to explain/critically examine the chemistry of transition metals, structure and bonding.*

Descriptive Inorganic Chemistry: (23 h)

Structure and bonding in polyhedral boranes and carboranes, electron count in polyhedral boranes – styx numbering, Wade‘s rules – polyhedral skeletal electron pair theory (PSEPT), synthesis of polyhedral boranes. Metal borides.

Organo compounds of Si, Ge, Sn and Pb; phosphates, phosphazenes and phosphines; metal-oxo compounds, calixarenes, cryptands and crown ethers in complexation chemistry, metal chalcogenides, sulfur-nitrogen compounds

Organometallic compounds of Li, Be, Mg and Hg

Chemistry of the elements of the second and third transition series – general overview of compounds having the metals in their common oxidation states; polyoxometallates of Mo and W; quadruple and quintuple M-M bonded compounds, methyltrioxorhenium (MTO); the Creutz-Taube complex; RuCl2(PPh3)3; osmium tetroxide; Vaska‘s compound; palladium complexes in the oxidation state 0; Pt(II,IV) linear chain compounds.

Molecular Symmetry and the Symmetry Groups: (12 h)

Symmetry elements and operations, classes of symmetry operations, symmetry point groups. Matrix notation for geometric transformations, reducible and irreducible representations, rules about irreducible representation as derived from great orthogonality theorem, relationship between reducible and irreducible groups, character tables.

Organometallic Chemistry-II: (10 h)

Synthesis, structure, bonding and reactivity of mono and polynuclear metal carbonyls. Substituted metal carbonyls. Vibrational spectra of metal carbonyls.

Types of M-C bonds, synthesis and reactivity of metal alkyls, carbenes, alkenes, alkynes, and arene complexes; metallocenes and bent metallocenes.

Recommended Books:

1. F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann; *Advanced Inorganic Chemistry*, 6th ed. Wiley, 1999

2. P.W. Atkins, T. Overton, J. Rourke, M. Weller, F. Armstrong; *Shriver & Atkins‘ Inorganic Chemistry*, 5th ed. Oxford University Press, 2010.

3. *Fundamental Concepts of Inorganic Chemistry*, Vols. 1-7, by A.K. Das and M. Das, CBS Publishers and Distributors, 2015

4. L. Smart, E. Moore, *Solid State Chemistry: An Introduction*, 2nd Ed. Nelson Thorns Ltd. 2004.

5. A. R. West, *Solid State Chemistry and Its Application*, Wiley Student Edition, John Wiley & Sons. 1998.

6. R. H. Crabtree, *Organometallic Chemistry of the Transition Metals 2nd Ed*. , John Wiley, 1993.

7. C.Elschenbroich, A. Salzer, *Organometallics: A Concise Introduction*, 2nd Ed. Wiley VCH, 1995.

LAB: (30 h)

1. Solid phase synthesis of coordination compounds (e.g. Reinecke salt, trans-bis-glycinatocopper(II)) and their properties.

2. Synthesis of metal nanoparticles (Cu, Ag, Au, etc.), characterization and investigation of their optical properties.

CHE8104M: Chemistry-VIII

Total lectures: 45(L+T) & 30 (P) Credits: 4 (Theory: 03, Lab: 01)

Course Objective: *In this course students will be introduced to different classes of organic compounds.*
Learning Outcome: *After completion of this course students will learn various classes of organic molecules-alkyl halides, aryl halides, alcohols, phenols, ethers, aldehydes and ketones.*

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

Alkyl and Aryl Halides: (10 h)

Alkyl Halide: Types of Nucleophilic Substitution (SN1, SN2 and SNi)reactions
Preparation: from alkenes *and* alcohols.
Reactions: hydrolysis, nitrite & nitro formation, nitrile & isonitrile formation. Williamson's ether synthesis: Elimination vs substitution.

Aryl Halide:
Preparation: (Chloro, bromo and iodo-benzene case): from phenol, Sandmeyer & Gattermann reactions.
Reactions (Chlorobenzene): Aromatic nucleophilic substitution (replacement by –OH group) and effect of nitro substituent. Benzyne Mechanism: KNH2/NH3 (or NaNH2/NH3). Reactivity and Relative strength of C-Halogen bond in alkyl, allyl, benzyl, vinyl and arylhalides.

Alcohols: (8 h)

Preparation: Preparation of 1º, 2ºand 3ºalcohols: using Grignard reagent, Ester hydrolysis, Reduction of aldehydes, ketones, carboxylic acid and esters.
Reactions: With sodium, HX (Lucas test), esterification, oxidation (with PCC, alk. KMnO4, acidic dichromate, conc. HNO3). Oppeneauer oxidation *Diols:* (Upto 6 Carbons) oxidation of diols. Pinacol-Pinacolone rearrangement.

Phenols& Ethers: (7 h)

Phenol:
Preparation: Cumene hydroperoxide method, from diazonium salts.
Reactions: Electrophilic substitution: Nitration, halogenation and sulphonation. Reimer-Tiemann Reaction, Gattermann-Koch Reaction, Houben–Hoesch Condensation, Schotten-Baumann Reaction.

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

Aldehydes and ketones (aliphatic and aromatic): **(12 h)**
(Formaldehye, acetaldehyde, acetone andbenzaldehyde)

Preparation: from acid chlorides and from nitriles.
Reactions – Reaction with HCN, ROH, $NaHSO_3$, NH2-G derivatives. Iodoform test. Aldol Condensation, Cannizzaro's reaction, Wittig reaction, Benzoin condensation. Clemensen reduction and Wolff Kishner reduction. Meerwein-Pondorff-Verley reduction.

Recommended Books:
1. T. W. Graham Solomons: *Organic Chemistry, John Wiley and Sons*.
2. Peter Sykes: *A Guide Book to Mechanism in Organic Chemistry*, Orient Longman.
3. I.L. Finar: *Organic Chemistry* (Vol. I & II), E. L. B. S.
4. R. T. Morrison & R. N. Boyd: *Organic Chemistry*, Prentice Hall.
5. Arun Bahl and B. S. Bahl: *Advanced Organic Chemistry,* S. Chand.
6. J. C. Kotz, P. M. Treichel& J. R. Townsend: *General Chemistry* Cengage Lening India Pvt. Ltd., New Delhi (2009).

7. B. H. Mahan: *University Chemistry* 3rd Ed. Narosa (1998).

8. R. H. Petrucci: *General Chemistry* 5th Ed. Macmillan Publishing Co.: New York (1985).

LAB: **(30 h)**

1. Purification of organic compounds by crystallization (from water and alcohol) and distillation.
2. Criteria of Purity: Determination of melting and boiling points.
3. Preparations: Mechanism of various reactions involved to be discussed.
4. Recrystallisation, determination of melting point and calculation of quantitative yields to be done.
(a) Bromination of Phenol/Aniline
(b) Benzoylation of amines/phenols
(c) Oxime and 2,4 dinitrophenylhydrazone of aldehyde/ketone

Recommended Books:
1. A.I. *Vogel: Textbook of Practical Organic Chemistry*, 5th edition, Prentice-Hall.
2. F. G. Mann & B. C. Saunders, *Practical Organic Chemistry*, Orient Longman (1960).

CHE8204M: Physical Chemistry-II

Total lectures: 45(L+T) & 30 (P) Credits: 4 (Theory: 03, Lab: 01)

Course objective: *Students will be introduced to the concepts of chemical kinetics, electrochemistry, molecular dynamics and fast reaction kinetics.*
Learning outcome: *Students will able to describe/examine the concepts and theories of chemical kinetics and electrochemistry, and the applications of molecular dynamics, fast reactions and energy storage.*

Advanced Chemical Kinetics: (8 h)

Steady state approximation and its applications, oscillating reactions, chemical Chaos, Belousov-Zhabotinski reaction, straight-chain reaction-hydrogen halogen reactions, alkane pyrolysis, Branching-chain reactions- the hydrogen-oxygen reaction, explosion limits, Enzyme catalyzed reactions, Michaelis-Menten mechanism- Lineweaver-Burk and Eadie plots, enzymeinhibiton.

Molecular Reaction Dynamics: (9 h)

Collisions of real molecules- trajectory calculations, Laser techniques, reactions in molecular beam, - reaction dynamics, Estimation of activation energy and calculation of potential energy surface- the transition state theory (TST) of bimolecular gaseous reactions, statistical and thermodynamic formulations. Comparison between TST and hard sphere collision theory, Theory of unimolecular reactions- Lindemann theory and its limitations, kinetics of reactions in solution-diffusion controlled and chemically controlled reactions, TST of reactions in solution- Bronsted and Bjerrum equation, effect of ionic strength, kinetic salt effect.

Study of Fast Reactions: (8 h)

Stopped flow technique, temperature and pressure jump methods, NMR studies in fast reactions, shock tube kinetics, relaxation kinetics, Linearized rate equation, relaxation time in single step fast reactions, determination of relaxation time.

Theories of Unimolecular Reactions: (6 h)

Drawbacks of Lindemann theory-Hinselwood modification, RRK theory, slaters treatment, RRKM theory.

Dynamic Electrochemistry: (8 h)

Ion-solvent interaction- the Born model, Thermodynamic parameters of ion solvent interactions-structural treatment, the ion-dipole model-its modifications, ion-quadrupole and ion-induced dipole interactions, Primary solution- determination of hydration number, compressibility method and viscosity-mobility method, Debye-Huckel theory of ion-ion interactions-derivation, validity and limitations, extended Debye-Huckel-Onsager equation. The random walk model of ionic diffusion-Einstein Smoluchowski reaction.

Theories of Electrical Interface: (6 h)

Electrocapillary phenomena- Lippmann equation, electron transfer at interfaces, polarizable and non-polarizable and nonpolarisable interfaces, Butler-Volmer equation, Tafel plot

Recommended Books:

1. P. Atkins and J. Paula, *Physical Chemistry*, 9th Edition, Oxford University Press, Oxford 2010.
2. I. R. Levine, *Physical Chemistry*, 6th Edition, McGraw Hill Education, 2011.
3. K. J. Laidler, *Chemical Kinetics*,3rd Edition, Pearson, 2012.
4. J. O. Bockris, A. K. N. Reddy, *Modern Electrochemistry Part 1, 2A and 2B*, 2nd Edition, Springer

5. A. J. Bard, L. R. Faulkner, *Electrochemical Methods Fundamentals and Applications*, 2nd edition, Willy India, 2006.

LAB: (30 h)

Kinetics by spectrophotometry, polarimetry and conductometry, Relative strength of two acids by conductance, Determination of a weak acid and a strong acid in mixture by potentiometry, Study of liquid-liquid phase diagram, Determination of fluoride by ion selective electrode, nitrate spectrophotometry, Determination of average molecular weight of a polymer by viscometry.

Study of excess adiabatic compressibility of binary system by ultrasonic interferometry, Simultaneous determination of CMC and partition equilibrium constant by spectroscopic method, Kinetics of the catalytic decomposition of H_2O_2 by manganese (IV) oxide, Determination of CMC by Du Nouy Tensiometry, Micellar catalysis by spectroscopy, Determination of pK_a by spectroscopy, Determination of stoichiometry and the stability constant of the complex formation, Determination of activation energy of reaction by polarimetry

Recommended Books:

1. Viswanathan, B., Raghavan, P. S. *Practical Physical Chemistry*, (Viva Books Pvt. Ltd., 2005).
2. James, A. M., Prichard, F. E. *Practical Physical Chemistry*, 3rd Edn., (Longman, 1974).
3. Jadav, J. B. *Advanced Practical Physical Chemistry*, (Krishna Prakashan, 2015).
4. Khosla, B. D.; Garg, V. C. & Gulati, A. *Senior Practical Physical Chemistry*, R. Chand & Co.: New Delhi (2011).
5. Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. *Experiments in Physical Chemistry 8th Ed.*; McGraw-Hill: New York (2003).