

Parvatibai Chowgule College of Arts & Science
(Autonomous)
Margao - Goa

MINUTES OF THE MEETING OF THE BOARD OF STUDIES IN CHEMISTRY

held on 22nd October 2016 at 10:00 A.M.

Part B: Resolutions/Recommendations that require consideration/approval of the Academic Council.

1. The syllabi of Semester V and VI are restructured and the elective courses have been combined or replaced. The BOS passed the resolution to restructure and replace the courses. The new structure is given as follows;

SEMESTER	CORE COURSES	ELECTIVE COURSES			
V	CHE-V Advanced Chemistry: Physical and Inorganic	CHE-V Heterocyclic and Organometallic Chemistry	CHE-V Selected Topics in Physical Chemistry	CHE-V Selected Topics in Inorganic Chemistry	CHE-V Environmental Chemistry
VI	CHE-VI Advanced Chemistry: Organic and Analytical	CHE-VI Principles and Applications of Spectroscopy	CHE-VI Instrumental Techniques in Chemistry	CHE-VI Nanomaterials and Solid State Chemistry	CHE-VI Xxxxxxx

2. The syllabi of Semester V and VI of the undergraduate courses were presented and discussed at the meeting. After corrections and changes suggested by the subject experts, the BOS resolved to pass the syllabi for the following undergraduate courses:

Sr. No.	CORE COURSE	Nature of the course	PG Level at which offered.
1	Advanced Chemistry: Physical and Inorganic	Core	
2	Advanced Chemistry: Organic and Analytical	Core	
3	Principles and Applications of Spectroscopy	Elective	
4	Selected Topics in Inorganic Chemistry	Elective	
5	Nanomaterials and Solid State Chemistry	Elective	
6	Environmental Chemistry	Elective	

3. The BOS has passed a resolution to design the following courses;

Sr. No.	CORE COURSE	Nature of the course	PG Level at which offered.
7.	Heterocyclic and Organometallic Chemistry	Elective	
8.	Selected Topics in Physical Chemistry	Elective	
9.	Instrumental Techniques in Chemistry	Elective	
10.	(Not decided)	Elective	

4. The BOS passed a resolution to design new experiments in some of the elective courses and to conduct a workshop in this regards.

The Chairperson thanked the members of the Board of Studies in Chemistry for their valuable contribution and active participation.

The meeting ended at 5:45 p.m. with a vote of thanks to the chair.

The following members of the Board of Studies in Chemistry were present for the meeting.

1. Dr. Roopa S. Belurkar - Chairperson
2. Dr. J. B. Fernandes -Member
3. Dr. J. S. Budkuley -Member
4. Dr. S. P. Kamat - Member
5. Shri. N. G. Rivonkar -Member
6. Dr. Sachin B. Kakodkar - Member
7. Dr. Manjita R. Porob -Member
8. Mrs. Manjita R. Porob - Member
9. Mrs. Padmini C. Panjekar - Member
10. Dr. Lactina R. Gonsalves -Member Secretary
11. Dr. Rohan K. Kunkalekar -Member
12. Dr. Sandesh T. Bugde -Member

Dr. Shirishbhai Patel, Dr. A. K. Srivastava and Dr. J. Seetharamappa conveyed their inability to attend the meeting.

Dr. G. K. Naik remained absent for the BOS meeting despite being present on the campus, thereby deferring from important academic duties as a member of BOS.

Dr. Roopa S. Belurkar
Chairperson
Board of Studies
Date: 11 /01/2017

Parvatibai Chowgule College of Arts and Science
(Autonomous)
DEPARTMENT OF CHEMISTRY
COURSE STRUCTURE
THREE YEAR B.Sc. DEGREE COURSE IN CHEMISTRY

SEMESTER	CORE COURSES		ELECTIVE COURSES			
I	CHE-I. C-1 General Physical and Inorganic Chemistry	CHE-II. C-2 General Organic and Inorganic Chemistry	---	---	---	---
II	CHE-II. C-3 Concepts in Physical and Analytical Chemistry	CHE-II. C-4 Concepts in Organic and Inorganic Chemistry	---	---	---	---
III	CHE-III. C-5 Comprehensive Chemistry –I	---	CHE-III. E-1 Name Reactions and Synthetic Methodologies	CHE-III. E-2 Industrial Chemistry	CHE-III. E-3 Surface Chemistry and Catalysis	CHE-III. E-4 Bioinorganic Chemistry
IV	CHE-IV. C-6 Comprehensive Chemistry –II	---	CHE-IV. E-5 Pharmaceutical Chemistry	CHE-IV. E-6 Polymer and Colloid Science	CHE-IV. E-7 Spectroscopic Techniques	CHE-IV. E-8 Chemistry of Natural Products
V	CHE-V. C-7 Advanced Chemistry – I (Physical & Inorganic Chemistry)	---	CHE-V. E-9 Heterocyclic Chemistry	CHE-V. E-10 Nanomaterials and solid state Chemistry	CHE-V. E-11 Organometallic Chemistry	CHE-V. E-12 Chemistry of main group elements
VI	CHE-VI. C-8 Advanced Chemistry-II : Organic and Analytical Chemistry	---	CHE-VI. E-13 Spectroscopic Methods in Organic Chemistry	CHE-VI. E-14 Environmental Chemistry	CHE-VI. E-15 Selected Topics in Inorganic Chemistry	CHE-VI. E-16 Solid State Chemistry



Parvatibai Chowgule College of Arts and Science

AUTONOMOUS

DEPARTMENT OF CHEMISTRY

SYLLABUS DRAFT

FOR THE UNDERGRADUATE COURSE IN CHEMISTRY

AT

T. Y. B. Sc. SEMESTER – V

FOR THE

ACADEMIC YEAR: 2017-2018

SEMESTER V

CORE COURSE

THEORY

Course Title: Advanced Chemistry I: Physical and Inorganic Chemistry

Course Code: CHE- I. C-7

Marks: 75

Credits: 03

Course Objectives:

1. To provide a basic understanding of the core areas of Physical Chemistry based on the theme of electrochemistry, spectroscopy etc.
2. To obtain a comprehensive understanding of the basic concepts in Inorganic Chemistry.
3. To generally provide practical skills to correlate with the theory.

Learning outcome

1. Will have a working knowledge of the main areas of Physical Chemistry, will develop critical thinking abilities and be able to work in chemical or related fields.
2. Will help to get better understanding about the basics of Physical and Inorganic Chemistry.
3. Will be able to carry out experiments with required skills.

SECTION I (PHYSICAL CHEMISTRY)

UNIT I: Molecular Spectroscopy

7L

Definition of spectrum. Electromagnetic radiation, quantization of different forms of energies in molecules : translational, rotational and electronic, Born Oppenheimer approximation, factors affecting line width and intensity.

Infrared spectroscopy

Hook's law, energy levels and transitions: Simple harmonic oscillator, anharmonic oscillator (derivations expected), Calculation of force constant, Stretching and bending vibrations, modes of vibration of diatomic, linear triatomic (CO_2) and non linear triatomic (H_2O) molecules, applications of IR spectroscopy.

Raman spectroscopy- Rayleigh and Raman scattering, Stokes and Antistokes lines. Mutual exclusion principle. Differences between Raman and IR spectroscopy

Numerical problems expected

UNIT II: Photochemistry

4L

Interaction of radiation with matter, difference between thermal and photochemical processes, Laws of photochemistry: Grothus – Drapper law, Stark – Einstein law, Jablonski diagram depicting various processes occurring in the excited state, qualitative description of fluorescence, phosphorescence, non- radiative processes (internal conversion, intersystem crossing), quantum yield, photosensitized reactions.

Numerical problems expected

UNIT III: Electrochemistry

7L

EMF of a cell and its measurements, concentration cells: electrode and electrolyte with and without transport, liquid junction potential and its measurement; applications of concentration cell: determination of ionic product of water, transport number of ions, solubility and solubility product.

Numerical problems expected

UNIT IV: Nuclear Chemistry

5L

Natural Radioactivity: kinetics of radioactive decay, half-life and average life of radioelements (derivations expected),

Measurement of radioactivity: GM counter, Scintillation counter

Artificial radioactivity: Chain reaction and conditions for its control.

Radioisotopes and their applications; radiolabelled reactions, radiocarbon dating, medicinal and agricultural field, hazards of radiation.

Numerical problems expected

SECTION II (INORGANIC CHEMISTRY)

UNIT V: Metal-Ligand Bonding in Transition Metal Complexes

11L

Principles and limitations of Valence bond theory, Crystal field theory (CFT) splitting of d- orbitals in octahedral, tetrahedral and square planar complexes. Crystal Field Stabilization Energy (CFSE), Measurement of 10 Dq for $[\text{Ti}(\text{H}_2\text{O})_6]^{3+}$ complex, Factors affecting 10 Dq, Spectrochemical series, Effect of crystal field splitting on properties of Octahedral complexes: Magnetic, Spectral.

UNIT VI: Electronic spectra of Transition Metal Complexes:

11L

Introduction, types of electronic transitions: The d-d transitions (d^1/d^9 and d^2/d^8), charge transfer transitions and ligand-ligand transitions, selection rules (Laporte orbital and spin), applications (ligand field strength, colour of complexes, *cis*-, *trans*- isomerism and geometry of complexes).

PRACTICALS

Course Title: Advanced Chemistry I: Physical and Inorganic Chemistry

Course Code: CHE- I. C-7

Marks: 25

Credits: 01

List of experiments:

Physical Experiments:

1. To determine the percent composition of acid mixture (strong and weak acid) by titrating against standard 0.1 N NaOH solution.
2. To determine the strength of mixture containing weak acid (CH_3COOH) and weak base (NH_4OH) by titrating against standard 0.1N NaOH solution
3. To determine the formal redox potential of $\text{Fe}^{2+}/\text{Fe}^{3+}$ system using standard 0.1N $\text{K}_2\text{Cr}_2\text{O}_7$ solution.
4. To determine the percent composition and amount of halide ions from their mixture (any two halides) using standard 0.1N AgNO_3 solution.
5. To determine the dissociation constant of weak monobasic acid (CH_3COOH) by titrating against standard 0.1N NaOH solution.
6. To study the acid hydrolysis of methyl acetate at three different temperatures and compare the energy of activation.

Any six

Inorganic experiments

1. Preparations of the following complexes. (2hours each)
 - a) $[\text{Ni}(\text{NH}_3)_6]\text{Cl}_2$
 - b) $[\text{Co}(\text{NH}_3)_3(\text{NO}_2)_3]\text{Cl}_3$
 - c) $[\text{Co}(\text{NH}_3)_6]\text{Cl}_3$
 - d) $\text{K}_3[\text{Al}(\text{C}_2\text{O}_4)_3]\cdot\text{H}_2\text{O}$
 - e) Preparation and estimation of Ti in $[\text{Ti}(\text{H}_2\text{O})_6]^{3+}$ complex.
2. Estimation of Ni in $[\text{Ni}(\text{NH}_3)_6]\text{Cl}_2$ gravimetrically

3. Estimation of Co in $[\text{Co}(\text{NH}_3)_6]\text{Cl}_3$ gravimetrically

REFERENCE BOOKS:

Physical Chemistry

TEXTBOOK:

1. Bahl B.S, et.al, 2004, "Essentials of Physical Chemistry" S. Chand & Co., New Delhi

ADDITIONAL READING:

2. Arnikar H.J.,1995, "Essentials of Nuclear Chemistry", Wiley-Eastern Ltd., New Delhi
3. Atkins P, et.al, 2006,"Physical Chemistry", Oxford University Press, New Delhi
4. Castellan, G.W,2002, "Physical Chemistry", Narosa Publishing House, New Delhi,
5. Kundu K. et.al,2003, "Physical Chemistry", S. Chand & Co., Ltd., New Delhi
6. Puri B.R et.al,2008,"Principles of Physical Chemistry", Vishal Publishing Company, Jalandhar
7. Raj Gurdeep, 2000 ,"Advanced Physical Chemistry", Goel Publishing House, Meerut
8. Srivastava A.K, et.al, 1989,"Essential of Nuclear Chemistry", S.Chand & Co, New.Delhi

Inorganic Chemistry

TEXTBOOK:

1. Atkins P, Overton T, Rourke J et.al, *Shriver and Atkins' Inorganic Chemistry*, 5th Edition, Oxford University Press.

ADDITIONAL READING:

2. Cotton F.A and Wilkinson G, *Basic Inorganic Chemistry*,Wiley Eastern Ltd.
3. Huheey J.E, Keiter E.A, Keiter R.L, Medhi O.K, *Inorganic Chemistry: Principles of Structure and Reactivity*, Pearson Edu.
4. Lee J.D, *Concise Inorganic Chemistry*, Wiley-India

SEMESTER V

ELECTIVE COURSES THEORY

Course Title: Heterocyclic Chemistry

Course Code: CHE- V. E-9

Maximum Marks: 75

Credits: 03

Course Objectives:

1. The main objective of this course is to study the chemistry of heterocyclic compounds.
2. This course gives an overview of different classes of heterocyclic compounds.
3. It includes physical, chemical properties and synthesis of most of the heterocyclic compounds.

Learning outcome:

1. Students will learn about important aspects with respect to heterocyclic chemistry.
2. Students will develop understanding with regards to reactivity of heterocyclic chemistry.
3. Students will learn efficient chemical synthesis involved in heterocyclic compounds.

UNIT I: Introduction to heterocyclic compounds **03L**

Classification and Nomenclature of aliphatic and aromatic heterocycles.

UNIT II: Aliphatic heterocycles **10L**

Structure and reactivity of nitrogen and oxygen containing aliphatic heterocycles. Methods of preparation and reactions of oxiranes, aziridines, tetrahydrofuran, pyrrolidine.

UNIT III: Five and six membered aromatic heterocycles **12L**

Structure and reactivity of five and six membered heterocycles: furan, pyrrole, thiophene and pyridine; comparison of basicity of pyrrole, pyridine & piperidine. Electrophilic substitution reactions of five and six membered heterocycles: General mechanism, mechanism of halogenation, nitration and reaction using acids (HCl, H₂SO₄ and HNO₃). Methods of preparation of furan, pyrrole, thiophene and pyridine. Nucleophilic substitution reactions of aromatic heterocycles.

UNIT IV: Condensed heterocycles **10L**

Structure and reactivity of condensed heterocycles like benzofuran, Indole, benzothiophene, quinoline and isoquinoline. Electrophilic and nucleophilic substitution reactions of condensed heterocycles: General mechanism and with examples. Oxidation and reduction of condensed heterocycles. Methods of preparation of benzofuran, Indole, benzothiophene, quinoline and isoquinoline.

UNIT V: Heterocycles containing more than one heteroatom **10L**

Classification of heterocycles containing more than one heteroatom. Reactions of 1,2-azoles, 1,3-azoles, oxazoles, imidazole, purines and pyrimidines: Reactions with electrophilic reagents, reactions with nucleophilic reagents. Methods of preparations of 1,2-azoles, 1,3-azoles, oxazoles, imidazole and purines.

PRACTICALS

Course Title: Heterocyclic Chemistry

Course Code: CHE- V. C-9

Marks: 25

Credits: 01

List of experiments:

1. Epoxidation of chalcones (2steps)
2. Synthesis of the Coumarins via Pechmann condensation
3. Synthesis of 3,4- dihydropyrimidin-2(1H)-ones by a one-pot three component cyclocondensation reaction of 1,3 dicarbonyl compound, aldehyde, and urea via Biginelli reaction
4. Synthesis of 1,3,5-trisubstituted pyrazoles (2steps)
5. Synthesis of benzimidazole from o-phenylenediamine and formic acid
6. Synthesis of 2-substituted benzoxazoles from 2-amino phenol and aromatic aldehydes.
7. Synthesis of quinoxaline derivatives
8. Synthesis of flavones via Baker-Venkataraman rearrangement (3steps)
9. Preparation of 2-phenyl indole via Fischer indole synthesis

REFERENCES:

TEXT BOOK

1. Joule J. A. and Mills K. **2010**. "*Heterocyclic Chemistry*". Wiley publications

ADDITIONAL READING:

1. Carey, F. C. and Giuliano, R. M. **2000**. "*Organic Chemistry*" Tata McGraw-Hill India.
2. Gilchrist T. **2007**. "*Heterocyclic Chemistry*". Pearson Education India
3. Smith, M. B and March, J . **2012**. "March's Advance organic Chemistry" Wiley publications.

THEORY

Course Title: Nanomaterials and Solid State Chemistry

Course Code: CHE-VI. E-10

Maximum Marks: 75

Credits: 3

Course Objectives:

The main objective of this course is to study the chemistry of nanomaterials, their synthesis, properties and applications. It also provides fundamental knowledge of solid state chemistry which involves reaction of solids and their electrical and magnetic properties.

Learning outcome:

1. Students will have a basic and concise knowledge of nanomaterials.
2. Students will develop skills in nanomaterial synthesis.
3. Will be able to understand characterization techniques in solid state chemistry.

UNIT I: Introduction and properties of nanomaterials

6L

Fundamentals: terminology and history, classification of nanomaterials, properties of nanomaterials: optical, magnetic, electronic, surface area, catalytic and mechanical.

UNIT II: Synthesis and characterization of nanomaterials

10L

Synthesis Approach with at least one example of each: Chemical methods (sol-gel, hydrothermal, sonochemical, microwave, precursor). Top down and bottom up, physical methods (mechanical methods, methods based on evaporation, sputter deposition, chemical vapour deposition), biological methods (using microorganism and plant extract).

Characterization techniques: electron microscopic techniques (SEM/TEM), diffraction techniques, spectroscopic (UV-Visible, magnetic measurement), BET surface area.

UNIT III: Applications of nanomaterials

6L

Energy, automobiles, sports, textile, cosmetics, medicinal, space, defence, engineering and catalytic.

Toxicity of nanomaterials

UNIT IV: Solid state chemistry

11L

Reactions of solids: tarnish reactions, decomposition reaction, solid-solid reactions, addition reactions, double decomposition reaction, electron transfer reaction, solid-gas reactions. Sintering.

Phase transformations in solids: structural change in phase transformation, Martensite transformation, temperature and pressure induced transformations, order-disorder transitions.

UNIT V: Electrical and magnetic properties of solids

12L

Electrical conductivity, insulators, semiconductor and conductors. Band theory of semiconductors, photo conductivity and ionic conductivity. Superconductivity, BCS theory, Meissner effect, types of superconductor.

Piezoelectric, ferroelectric materials and applications.

Introduction to magnetism, behavior of substance in a magnetic field, magnetic moments, diamagnetism, paramagnetism, experimental determinations of susceptibility, ferromagnetism, antiferromagnetism, ferrimagnetism, magnetizations of a ferromagnetic substance.

PRACTICALS

Course Title: Nanomaterials and Solid State Chemistry

Course Code: CHE-VI. E-10

Maximum Marks: 25

Credits: 01

List of Practicals:

1. Synthesis of silver nanoparticles by chemical method.
2. Synthesis of ZnO nanomaterials.
3. Synthesis of CdS nanomaterials.
4. Synthesis of nanoparticles using plant extract (metal/ metal oxides).
5. To find out particle size using SEM/TEM data.
6. To study the X-ray diffraction pattern of given sample (Phase and particle size).
7. Preparation of zinc oxalate dihydrate and analysis of its TG/DTA pattern.
8. To prepare mixed metal oxide of Zn and Fe using co-precipitation technique.
9. To prepare mixed metal oxide of Zn and Fe using precursor technique.
10. Measurements of electrical and magnetic properties of pure and mixed metal oxides.

REFERENCE BOOKS:

TEXTBOOK:

1. Atkins P. W., Overton T. L., Rourke J. P., Weller M. T. and Armstrong F. A., *Shriver and Atkins Inorganic Chemistry*, Oxford University press.

ADDITONAL READING:

1. Keer H. V., *Principles of Solid State Chemistry*, New Age International Publishers,
2. Kulkarni S. K., *Nanochemistry, Principles and Practices*, Capital publishers.
3. Poole C. P. and Owens F. J., *Introduction to Nanotechnology*, John-Wiley and Sons.
4. Rao M. B. and Reddy K. K., *Introduction to Nanotechnology*, Campus books International.
5. West A. R., *Solid State Chemistry and its Applications*, John-Wiley and Sons.

THEORY

Course Title: Organometallic Chemistry

Course Code: CHE- III. E-11

Maximum Marks: 75

Credits: 03

Course Objectives:

To provide knowledge of fundamental content in the area of organometallic chemistry and impart practical skills so that the student will be able to integrate the knowledge with critical thinking to solve problems.

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

1. Use the basic principles of chemistry and molecular orbital theory to describe chemical bonding and structure of organometallic compounds and describe the structure and behaviour of organometallic compounds.
2. Explain and predict the chemical behavior and reactivity of organometallic compounds.
3. Describe and explain catalytic processes using an organometallic compound as a catalyst and explain how organometallic compounds are used as catalysts in organic synthesis.

UNIT I: Introduction to organometallic chemistry

08L

Definition, classification of organometallic compounds, Nomenclature, ligands, concept of hapticity of organic ligands, 18 electron rule, EAN concept, electron counting and oxidation states in complexes. General methods of preparation with one example of each (direct combination, reductive carbonylation, thermal and photochemical decomposition) and general properties of organometallic compounds of 3d series.

UNIT II: Metal carbonyls

10L

Classification of metal carbonyls; Mononuclear metal carbonyls: Preparation, properties, structure and bonding of $\text{Ni}(\text{CO})_4$, $\text{Fe}(\text{CO})_5$, $\text{Cr}(\text{CO})_6$ using VBT; Polynuclear metal carbonyls: Preparation, properties, structure and bonding of $\text{Co}_2(\text{CO})_8$, $\text{Mn}_2(\text{CO})_{10}$, $\text{Fe}_2(\text{CO})_9$ and $\text{Fe}_3(\text{CO})_{12}$. π -acceptor behaviour of CO (MO diagram of CO), synergic effect and use of IR data to explain structure and bonding in metal carbonyls.

UNIT III: Metallocenes

09L

Sandwich compounds, Ferrocene: Preparation and reactions (acetylation, alkylation, metallation, Mannich Condensation etc.). Structure and aromaticity, comparison of aromaticity and reactivity with benzene. Synthesis and reactivity of cyclopentadienyl compounds, bonding in bis(cyclopentadienyl) complexes, Fluxional behaviour of metallocenes. Metal-metal bonding and metal clusters: structure of clusters, electron counting in clusters, synthesis of clusters.

UNIT IV: Organometallic compounds of Main group elements

09L

Preparation, properties, reactions and structure of alkyls and aryls of Group 1 elements (Li, Na); Group 2 elements (Be, Mg); Group 13 elements (B, Al), Group 14 (Sn, Pb). Alkyls and aryl compounds of Ti, Zn and Hg

UNIT V: Reactivity of organometallic compounds

09L

Reactions of organometallic compounds: Ligand substitution, Oxidative addition and reductive elimination, σ -bond metathesis, 1,1-migratory insertion reactions, 1,2-insertions and β -hydride elimination. Catalysis by organometallic compounds: Alkene hydrogenation with Wilkinson's catalyst, hydroformylation, Ziegler-Natta catalysts.

PRACTICALS

Course Title: Organometallic Chemistry

Course Code: CHE- III. E-11

Maximum Marks: 25

Credit: 01

List of practicals:

1. Synthesis of Bromo(4-tert-butylpyridine)cobaloxime
2. Synthesis of Ethyl(4-tert-butylpyridine) cobaloxime
3. Preparation of chloro(pyridine) *bis* (dimethylglyoximate) cobalt(III)
4. Preparation of bromo (pyridine) bis (dimethylglyoximate) cobalt (III)
5. Preparation of Grignard reagents with different alkyl/aryl substituent.
 - i. phenyl magnesium bromide
 - ii. phenyl magnesium chloride
 - iii. methyl magnesium iodide
6. Preparation of alcohol using Grignard reagent (or any other Grignard reaction)
7. Structure analysis of metal-carbonyls based on IR data.
8. Metal complexes with triphenyl phosphine (minimum 4 hrs)
 - i. $\text{Co}(\text{PPh}_3)\text{Cl}_2 \cdot 2\text{H}_2\text{O}$
 - ii. $\text{Ni}(\text{PPh}_3)\text{Cl}_2 \cdot 2\text{H}_2\text{O}$

REFERENCE BOOKS:

TEXTBOOK:

1. Atkins P, Overton T, Rourke J et.al, *Shriver and Atkins' Inorganic Chemistry*, 5th Edition, Oxford University Press.

ADDITIONAL READING:

2. Cotton F.A and Wilkinson G, *Basic Inorganic Chemistry*, Wiley Eastern Ltd.
3. Huheey J.E, Keiter E.A, Keiter R.L, Medhi O.K, *Inorganic Chemistry: Principles of Structure and Reactivity*, Pearson Edu.
4. Lee J.D, *Concise Inorganic Chemistry*, Wiley-India



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SEMESTER VI

CORE COURSE

THEORY

Course Title: Advanced Chemistry: Organic and Analytical

Course Code: CHE- VI. C-8

Marks: 75

Credits: 03

Course Objectives:

1. To provide a basic understanding of the core areas of Organic and Analytical Chemistry.
2. To understand principles, techniques and applications of separation techniques
3. To use separation techniques for qualitative and quantitative analysis.

Learning outcome

1. Will learn to write mechanisms with stereochemistry.
2. Will learn principles of separation and its applications.
3. Will have practical knowledge of chromatographic techniques.
4. Will be able to carry out experiments with required skills.

SECTION I (ORGANIC CHEMISTRY)

UNIT I: Mechanism and stereochemistry of addition, substitution and elimination reactions

7L

Mechanism and stereochemistry of (i) Addition of halogens acids (HX) and halogen (X_2) to open chain alkenes. Markownikoff's and anti-Markownikoff's addition. (ii) S_N1 , S_N2 , S_{Ni} , substitutions and (iii) E1, E2 and E1cb elimination reactions.

UNIT II: Organic Compounds containing Nitrogen

6L

Preparation of nitroalkanes and nitroarenes. Chemical reactions of nitroalkanes. Mechanisms of nucleophilic substitution in nitroarenes and their reductions in acidic, neutral and alkaline media. Picric acid: preparation and properties. Structure and nomenclature of amines, physical properties. Structural features affecting basicity of amines. Amine salts as phase-transfer catalysts. Preparation of alkyl and aryl amines by reduction of nitro compounds and nitriles, reductive amination of carbonyl compounds, Gabriel phthalimide reaction and Hofmann rearrangement.

UNIT III: Carbohydrates

6L

Classification and nomenclature. Monosaccharides: General reactions, chain lengthening by Killiani-Fischer synthesis and chain shortening by Ruff degradation of aldoses, mechanism of osazone formation. Configuration of monosaccharides with reference to glucose. d(+)/l(-) and D/L systems of nomenclature. Interconversion of glucose to fructose and glucose to mannose. Cyclic structure of D(+)-glucose. Mechanism of mutarotation. Formation of glycosides, ethers and esters. Structure of sucrose and inversion of cane sugar.

UNIT IV: Chemistry of Organosulfur and organophosphorus compounds

4L

Nomenclature and classification of Organosulfur compounds. Methods of preparation and chemical reactions of thiols, disulfides and sulphonic acids. Nomenclature and classification of organophosphorus compounds. Preparation of phosphines. Phosphorous ylides and their general methods of preparation. Wittig reaction and its synthetic applications.

SECTION II (ANALYTICAL CHEMISTRY)

UNIT V: Solvent Extraction

05L

Principle, efficiency of extraction, percentage extraction, complexing agents in solvent extraction, separation factor, types of extraction, applications of solvent extraction

(Numericals expected)

UNIT VI: Chromatographic techniques

17L

Principle, classification of chromatographic techniques

Column Chromatography: Principle, technique and applications

Paper chromatography: Principle, technique and applications

Thin layer chromatography: Principle, technique and applications

Theory of chromatographic separation: Distribution equilibrium, rate of travel, retention time, retention volume and relative retention.

Ion exchange chromatography: Principle, classification of ion exchangers. Factors affecting the distribution of ions between the resin and the solution, ion exchange capacity, applications of ion exchange chromatography

Gas chromatography: Principle, instrumentation, and applications. Comparison of GSC and GLC

HPLC: Principle, instrumentation and applications

Hyphenated techniques: GC-MS and LC-MS

(Numericals expected)

PRACTICALS

Course Title: Advanced Chemistry II

Course Code: CHE- I. C-8

Marks: 25

Credits: 01

List of experiments:

ORGANIC CHEMISTRY EXPERIMENTS:

Organic mixture separation, purification of individual compounds and qualitative analysis of separated compound.

At least 08 mixtures of compounds:

Solid-solid, 04 mixtures

Solid-liquid, 02 mixtures

Liquid-liquid, 02 mixtures

Note: 1 gm of solid-solid mixture to be analyzed on small scale. 3-4 ml of liquid to be added in mixture.

ANALYTICAL CHEMISTRY EXPERIMENTS:

1. To estimate sodium from NaCl using cation exchanger resin
2. To separate metal ions by paper chromatography and determine retardation factor
3. To study separation of organic compounds by TLC
4. To estimate magnesium from Zn^{2+}/Mg^{2+} mixture by using an anion exchanger resin
5. To estimate zinc from Zn^{2+}/Mg^{2+} mixture by using an anion exchanger
6. To determine the equilibrium constant for the reaction $KI + I_2 = KI_3$
7. To determine partition coefficient for the distribution of iodine between CCl_4 and water
8. To separate a mixture of carboxylic acid and neutral compound by using solvent extraction technique.

9. To determine distribution coefficient for the partition of benzoic acid between methylene dichloride and water

REFERENCE BOOKS:

Organic Chemistry TEXT BOOK

1. Morrison, R. T., etal. **2010**. "Organic Chemistry". Pearson Publications, Noida India.

ADDITIONAL READING

1. Bruice, P. Y. **2015**. "Organic Chemistry". Pearson Publications, Noida India.
2. Carey, F. C., etal. **2012**. "Organic Chemistry". Tata McGraw-Hill India.
3. Finar, I. L. **2013**. "Organic Chemistry". Volume 1. Pearson Publications, Noida India.

ANALYTICAL CHEMISTRY

1. Christian, G. D. "Analytical Chemistry". 5th edition. John Wiley publications
2. Skoog D.A., West D. M. and Holler F. J.; Fundamentals of Analytical Chemistry, 4th Saunders College Publishing

SEMESTER VI

ELECTIVE COURSE THEORY

Course Title: Spectroscopic Methods in Organic Chemistry

Course Code: CHE-VI. E-13

Maximum Marks: 75

Credits: 03

Course Objectives:

1. To understand the importance of spectroscopy in organic chemistry.
2. To understand principles and applications of UV-Visible spectroscopy, IR Spectroscopy, Nuclear Magnetic Resonance and Mass Spectrometry.
3. To learn structure elucidation of organic compounds based on spectral data.

Learning outcome:

1. Will be able to do spectral analysis of organic compounds.
2. Will learn theory of important spectroscopic techniques.
3. Will be able to elucidate structures of organic compounds based on spectral data.
4. Will be able to operate an UV-visible spectrometer.

UNIT I: Introduction to spectroscopy

3L

Nature of electromagnetic radiation: wave length, frequency, energy, amplitude, wave number, and their relationship, different units of measurement of wavelength frequency, different regions of electromagnetic radiations, Regions of electromagnetic radiation. Interaction of radiation with matter: absorption, emission, fluorescence and scattering, types and advantages of spectroscopic methods.

UNIT II: UV-Visible Spectroscopy

6L

Ultraviolet (UV) absorption spectroscopy: Absorption laws (Beer-Lambert law), molar absorptivity, presentation and analysis of UV spectra, types of electronic transitions, effect of conjugation. Concept of chromophores and auxochromes, bathochromic, hypsochromic, hyperchromic and hypochromic shifts. UV spectra of conjugated dienes and enones, Woodward-Fieser rules for calculation of UV maxima of the above two systems.

Numerical problems expected

UNIT III: Infra Red (IR) absorption spectroscopy

6L

Molecular vibrations, Hooke's law, selection rules, intensity and position of IR bands, measurement of IR spectrum, functional group region, finger print region and its use to establish identity, applications to determine purity, to study progress of chemical reactions and hydrogen bonding. Characteristic absorptions bands of various functional groups and interpretation of IR spectra of organic compounds. Structure elucidation by using UV and IR spectral data is expected.

UNIT IV: Proton Magnetic Resonance (^1H NMR) spectroscopy

13L

Introduction to NMR Spectroscopy, types of protons: equivalent, non-equivalent, homotopic, enantiotopic and diastereotopic protons, NMR Spectrometer (block diagram), nuclear shielding and deshielding, chemical shift and molecular structure, spin-spin splitting and coupling constants, intensity of peaks, interpretation of ^1H NMR spectra of simple organic molecules. Structure elucidation of organic compounds using ^1H NMR spectral data is expected.

UNIT V: ^{13}C Nuclear Magnetic Resonance

10L

Number of signals, splitting of signals, proton coupled and decoupled spectra, off resonance decoupled spectra. ^{13}C NMR chemical shifts, identification of hybridization of carbons and nature of functionalization. Structure elucidation of organic compounds using ^{13}C NMR spectral data is expected.

UNIT VI: Mass Spectrometry

7L

Instrumentation, definitions of parent or molecular ion peak and base peak. Isotope effect with respect to alkyl halides. Fragmentation of ketones: α -cleavage and Mc-Lafferty rearrangement.

[Structure elucidation of organic compounds using Mass, UV, IR, ^1H NMR and ^{13}C NMR spectral data is expected]

PRACTICALS

Course Title: Spectroscopic Methods in Organic Chemistry

Course Code: CHE-VI. E-13

Maximum Marks: 25

Credits: 01

List of experiments:

1. Calculate UV maxima for given organic structure and match it with the given spectra of organic compounds.
2. Match the given set of organic compounds with the given set of spectra. List: Alkane, alkene, alcohol, ether, amine, carboxylic acid, ester and amides.
3. Verify Bathochromic, hypsochromic, hyperchromic and hypochromic shifts in phenol and aniline using UV-Vis spectrometer.
4. Identification of organic compounds based on given IR spectra of organic compounds.
5. On basis of IR spectra, distinguish between the given set of organic compounds. (set of 2 compounds \times 3).
6. Identify the compounds based on given Mass Spectra. List: Alkane, alkene, alcohol, ether, amine, carboxylic acid, ester and amides.
7. Give the fragmentation patterns for the given mass spectra of organic compounds.
8. Compare relative abundance of isotopes of halogen containing compound.
9. Determination of organic compound using given set of ^1H NMR data.
10. Determination of organic compound using given ^1H NMR spectrum.
11. Assigning the chemical shift values to the peaks of given ^1H NMR spectrum of organic compounds.
12. Determination of organic compound using given set of ^{13}C NMR data.
13. Assigning the chemical shift values to the peaks of given ^{13}C NMR spectrum of organic compounds.
14. Assigning the chemical shift values to the peaks of given ^1H NMR spectrum of organic compounds.
15. Identification of organic compounds based on given spectroscopic information.

REFERENCE BOOKS:

TEXTBOOKS:

1. Silverstein, R. M., et. al. **2015**. "*Identification of Organic Compounds*". Wiley publications

REFERENCE:

1. Kalsi, P. S. **2007**. "*Spectroscopy of Organic compounds*". New Age International (P) Ltd. New Delhi.
2. Morrison, R. T., et. al. **2010**. "*Organic Chemistry*". Pearson Publications, Noida India.
3. Pavia, D. L., et. al. **2008**. "*Introduction to Spectroscopy*". Cengage Learning.

THEORY

Course Title: Environmental Chemistry

Course Code: CHE-VI. E-14

Maximum Marks: 75

Credits: 03

Course Objectives:

1. To provide a basic interdisciplinary introduction to environmental challenges
2. To obtain a comprehensive understanding of the basic concepts in analytical instrumental techniques
3. To generally provide practical skills to correlate with the theory.

Learning outcomes

The course provides understanding how:

1. pollution affects our environment
2. knowledge of chemistry can be used to solve problems.
3. instrumental techniques can be used for chemical analysis of pollutants.

UNIT I: Introduction

7L

Atmosphere: Composition, Structure, properties vertical temperature behavior, lapse rate and temperature inversion.

- a) **Air pollution:** Introduction, classification of pollutants, sources, control, effect w.r.t. oxides of Nitrogen, Carbon and Sulphur, Photochemical smog, acid rain and Green House effect
- b) **Water pollution:** Chemical, physical and biological characteristics of water pollution, specific and Nonspecific characterization of water. DO, BOD, COD and chlorine demand, typical water treatment and waste water treatment. Importance of buffer and buffer index in waste water treatments.
- c) **Chemistry of soils:** Macro- and micro-nutrients in soil, chemistry of minerals of soil forming rocks. Toxic elements in soil including those are in trace quantities, pollutant materials.

UNIT II: Sampling of Pollutants

5L

Sampling of air pollutants:

- a) Absorption in liquids
- b) Adsorption on solids: cold trapping adsorption and collection of particulates.

Sampling of water pollutants: sampling and sample preservation.

Sampling of solids: sample size, equipment and methods of sampling, Auger sampler, tube sampler.

UNIT III: Chemistry of atmosphere and soil

7L

Reactions in the atmosphere: a) formation in the atmosphere b) reaction of hydroxyl radical with trace gases and as sources of hydroperoxy radical and hydrogen peroxide.

The methane cycle.

Chemistry of minerals and soil forming rocks, trace material in soil.

Macronutrients : N, P,K in soil.

Pollutants in soil

UNIT IV: Adverse effects of specific pollutants**3L**

Effects of Hg, Pb and nitrites on humans and other living organisms.

Oil Spill: Biological and physical effects.

Acid, mine and drainage: Reactions of FeS₂ (pyrites), Cr, As and F.

UNIT V: Ozone Chemistry**06L**

Major atmospheric species involved in ozone formation and destruction.

Some major chemical reactions in the troposphere associated with ozone.

Stratospheric ozone: pollutants destroying stratospheric ozone layer

Species destroying ozone layer: a) catalytic NO, b) photo dissociation of CFCs, c) catalytic role of chlorine, and d) combined chain reaction

The ozone holes

Ozone layer and the green house effect.

UNIT VI: Techniques of water treatment**7L**

Water conditioning

- a) Treatment of water for municipal purpose: important process involved in purification of water.
- b) Treatment of water for Industries: removal of hardness of water Clark's method, use of ion exchange resins. Solid waste management
- c) Classification of solid wastes, types of waste of origin.
- d) Solid waste management method: (i) Utilisation, (ii) Recovery, (iii) Reuse (iv) Recycling of wastes/residues, (v) Recycling avoidance of solid waste.
- e) Use of Remote Sensing in Environmental Management.

UNIT VII: Optical and radiochemical techniques**3L**

1. Turbidimetry and Nephelometry: introduction, basic principle
2. Isotope dilution analysis: principles and applications
3. Neutron activation analysis: principles and applications

UNIT VIII: Application of instrumental techniques in environmental and chemical analysis **7L**

1. Air analysis: (a) SO₂, (b) H₂S, c) CO and d) CO₂.
2. Water analysis: a) determination of organic loadings b) determination of toxic metal ions by
 - (i) Atomic Absorption Analysis,
 - (ii) Atomic Emission techniques: mass spectrometry
3. Soil/Sediment analysis:
 - a) Bulk density, b) Specific gravity, c) Moisture content d) Water holding capacity e) Conductivity f) Alkalinity, and g) detection of Sulphate, calcium and iron

PRACTICALS

Course Title: Environmental Chemistry

Course Code: CHE-VI. E-14

Maximum Marks: 25

Credits: 01

List of Practicals:

1. Determination of sodium in water: ion exchange method
2. Determination of Total solids, Total dissolved solids and total suspended solids and its significance.
3. Determination of chlorine content in tap water samples: Mohr's method
4. Determination of acidity and alkalinity in water samples.
5. Determination of total, permanent and temporary hardness of water sample
6. Determination of DO of water sample
7. Determination of polluting elements such as Pb, Hg and As in water.
8. Analysis of Mn in a water sample by visual titrimetry.
9. Analysis of different types of soil- pH, conductivity, alkalinity
10. Determination of nitrite in water : colorimetric method
11. Determination of COD of water samples
12. Determination of BOD of water samples
13. Determination of phosphate: Colorimetric method

REFERENCE BOOKS:

1. Christian G. D., 5th edition , "Analytical Chemistry ", Wiley publication
2. De, A. K, 1995 "Environmental Chemistry", Wiley eastern Ltd.
3. Iqbal, S.A. et. al, 1995, " Chemistry of Air and Air Pollution", Discovery Publishing House, New Delhi
4. Katyal Jimmy et. al, 1993, "Environmental Pollution", Anmol Publications, New Delhi
5. Manahan, S.E. 1994, "Environmental Chemistry" Lewis Publishers
Neil, P. O 2007, "Environmental Chemistry", Blackie Academic & Professional
6. Raghuraman, K. et al, 4th edition, " Basic Principles of Analytical Chemistry", sheth publishers
7. Schroede, E.D, 1997, "Water & waste water treatment", Mc. Graw Hill
8. Skoog et. al, 4th International edition , "Principles of Analytical Chemistry"
9. Trivedi P.R. et. al, 1st edition "Environmental Water and Soil Analysis",
10. Akashdeep Publishing House, New Delhi
11. Tyagi, O.D. et. al, 1992, "A Text Book Of Environmental Chemistry" Anmol Publications, New Delhi
12. Vanloon G.W. et. al, 2003, "Environmental Chemistry", Oxford University Press

THEORY

Course Title: Selected Topics in Inorganic Chemistry

Course Code: CHE- III. E-15

Maximum Marks: 75

Credits: 03

Course Objectives:

To provide knowledge of fundamental content in various areas of inorganic chemistry and impart practical skills so that the student will be able to integrate the knowledge with critical thinking to solve problems.

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

4. encourage students to analyze and integrate concepts relevant to graduate level Inorganic chemistry.
5. understand the bond formation of compounds with special reference to MOT and CFT.

UNIT I: Inorganic Polymers

8L

Definition, properties, classification (condensation, addition and coordination), preparation, structure and bonding and applications of polymers containing Boron (borazine), phosphorous (phosphazenes), silicon (silicones), sulfur (S_4N_4 , thiazyl halides).

UNIT II: Magnetic Properties of Transition Metal Complexes

7L

Types of magnetic behaviour, magnetic susceptibility, effect of temperature on magnetic properties, Curie temperature, Neel temperature, Curie-Weiss law. Methods of determining magnetic susceptibility, Guoy's balance, spin only formula, calculation of magnetic moment of transition metal ions, application of magnetic moment data for 3d-metal complexes.

UNIT III: Thermodynamic and Kinetic Aspects of Metal Complexes

12L

Thermodynamic and kinetic stability of metal complexes, equilibrium constants, formation constants, lability, inert complexes, factors affecting the stability, substitution reactions in tetrahedral and octahedral complexes. Electron transfer reactions- inner sphere mechanism and outer sphere mechanism, Trans effect with respect to square planar complexes.

UNIT IV: Materials Chemistry

10L

Zeolites: types, structure and applications.

Composite materials: Metal-organic frameworks (MOF's); structure, ligands, applications.

Molecular materials: Fullerenes, liquid crystals, molecular magnets.

Superconductors: discovery, critical temperature, Meissner effect, types of superconductors.

Corrosion: response of material to chemical environments, galvanic corrosion and other forms of corrosion.

Prevention methods.

UNIT V: Molecular Symmetry

8L

Symmetry elements and operations: Centre of symmetry, Rotation axis, Mirror plane, rotation-reflection axis, Identity element. Point groups, Identifying symmetry elements and point group in molecules. (examples to be solved)

PRACTICALS

Course Title: Selected Topics in Inorganic chemistry

Course Code: CHE- III. E-15

Maximum Marks: 25

Credit: 01

List of practicals

1. Separation and Determination of transition metal ions
 - a) Separation of Mg^{2+} and Zn^{2+} by ion exchange and its estimation (4 hrs)
 - b) Separation of Cd^{2+} and Zn^{2+} by ion exchange and its estimation (4 hrs)
2. Determination of stability constant of complex ions in solution
 - a) Fe(III) – salicylic acid complex (Job's Method)
 - b) Fe(II) – 1,10-phenanthroline
3. Determination of instability constant for the reaction between Ag^+ and NH_3
4. Determination of instability constant for the reaction between Cu^{2+} and en
5. Estimation of Ca in compounds containing calcium.
6. Estimation of Ni in compounds containing nickel.
7. Estimation of Cu in compounds containing copper.
8. Estimation of metal ions in mixed metals compound.

REFERENCE BOOKS:

TEXTBOOKS:

1. Atkins P, Overton T, Rourke J et.al, *Shriver and Atkins Inorganic Chemistry*, Oxford University Press.

ADDITIONAL READING:

1. Lee J.D, *Concise Inorganic Chemistry*, Wiley-India
2. Huheey J.E, Keiter E.A, Keiter R.L, Medhi O.K, *Inorganic Chemistry: Principles of structure and reactivity*, Pearson Edu., 1993
3. Cotton F.A and Wilkinson G, *Basic Inorganic Chemistry*, Wiley Eastern Ltd, 1993
4. Puri B.R, Sharma L.R, Kale K.C, *Principles of Inorganic Chemistry*, Vallabh Publications.