Rayat Shikshan Sanstha's
Yashavantrao Chavan Institute of Science, Satara
(Autonomous)

Department of Chemistry

Postgraduate Programme

Two Year Degree Program in Chemistry

M. Sc. I - Chemistry

Choice based credit system Syllabus

(To be implemented from academic year 2021-22)

1. Title: Chemistry (Inorganic, Physical, Organic and Analytical)

2. Year of Implementation:

The syllabus will be implemented from June, 2021 onwards.

3. Preamble:

This syllabus is framed to give advanced knowledge of Chemistry to postgraduate students at first year of two years of M.Sc. degree course.

The goal of the syllabus is to make the study of chemistry , interesting and encouraging to the students for higher studies including research.

The new syllabus is based on a basic and applied approach with vigor and depth. At the same time precaution is taken to make the syllabus comparable to the syllabi of other universities and the needs of industries and research.

The syllabus is prepared after discussion at length with number of faculty members of the subject and experts from industries and research fields.

The units of the syllabus are well defined, taking into consideration the level and capacity of students.

4. GENERAL OBJECTIVES OF THE COURSE:

1. To educate and prepare post graduate students from rural and urban area who will get employment on large scale in academic institutes, R & D and Quality control laboratories of Indian chemical/pharmaceutical industries as well as multinational and forensic Laboratories.
2. To provide students with broad theoretical and applied background in all specialization of Chemistry with emphasis on qualitative and quantitative technique.
3. To provide broad common frame work of syllabus to expose our young graduates to the recent and applied knowledge of interdisciplinary branches of chemistry involving applied organic, inorganic, physical, analytical, industrial, pharmaceutical, polymer, nano science &technology.
4. To conduct lesser written tests and to encourage on non-written tests.
5. To focus on encouraging students to conduct various academic activities like midterm tests, online tests, open book tests, tutorial, surprise test, oral, seminar, assignments and seminar presentation.

Learning outcomes:

1. A graduate with a Master's degree in Chemistry has in-depth and detailed functional knowledge of the fundamental theoretical concepts and experimental methods of chemistry.
2. The graduate has expert knowledge of a well-defined area of research within chemistry. The graduate has specific skills in planning and conducting advanced chemical experiments and applying structural-chemical characterization techniques. Skilled in examining specific phenomena theoretically and/or experimentally, the graduate is able to contribute to the generation of new scientific insights or to the innovation of new applications of chemical research.

5. duration : One Year

6. Pattern : Semester

7. Medium of Instruction: English

8. STRUCTURE OF COURSE: SEMESTERWISE

Semester	Paper No.	Title	Total No. of lectures/practicals	Credits
Sem I	**Theory Course**			
	MDCT-101	Inorganic Chemistry	60 hrs	4
	MDCT-102	Organic Chemistry	60 hrs	4
	MDCT-103	Physical Chemistry	60 hrs	4
	MDCT-104	Analytical Chemistry	60 hrs	4
	Practical Course			
	MCP-105	Chemistry Practical-I	15 Practicals	4
	MCP-106	Chemistry Practical-II	15 Practicals	4
Sem II	**Theory Course**			
	MCT-201	Inorganic Chemistry	60 hrs	4
	MCT-202	Organic Chemistry	60 hrs	4
	MCT-203	Physical Chemistry	60 hrs	4
	MCT-204	Analytical Chemistry	60 hrs	4
	Practical Course			
	MCP-206-III	Chemistry Practical-III	15 Practicals	4
	MCP -207-IV	Chemistry Practical-IV	15 Practicals	4
			Total Credits	**48**

- The semester examination will be conducted at the end of each Semester (both theory and practical examination)
- Theory paper will be of 60 marks each and 40 marks for internal evaluation test conducted in the mid of the term. Two practicals will be of 100 marks each.
- Question papers will be set in the view of the entire syllabus and preferably covering each unit of the syllabus.

9. Evaluation Pattern For M. Sc. I

Paper code	Theory	Practical	
	ESE	ISE	Total
MCT- 101 & MCT - 201	60	ISE-I = 10 ISE-II = 10 (Online test) Activity = 20 (Book review) Total = 40	100
MCT- 102 & MCT - 202	60	ISE-I = 10 ISE-II = 10 (Online test) Activity = 20 (CIII online course) Total = 40	100
MCT – 103 & MCT- 203	60	ISE-I = 10 ISE-II = 10 (Online test) Activity = 20 (Survey/Seminar) Total = 40	100
MCT -104 & MCT - 204	60	ISE-I = 10 ISE-II = 10 (Online test) Activity = 20 (Group discussion/Innovative idea presentation) Total = 40	100
	240	160	400
Practical paper – I MCP -105, MCP- 106	60	Journal = 10 Student performance = 10 Activity = 20 (case study/survey report) Total = 40	100
Practical paper – II MCP-205, MCP- 206	60	Journal = 10 Student performance = 10 Activity = 20 (model presentation/project part I) Total = 40	100
Total	360	240	600

Laboratory Safety Equipment's: Part: I

Personal Precautions:

All persons must wear safety Goggles at all times.

1. Must wear Lab Aprons/Lab Jacket and proper shoes.
2. Except in emergency, over – hurried activities is forbidden.
3. Fume cupboard must be used whenever necessary.
4. Eating, Drinking and Smoking in the laboratories strictly forbidden.

Part: II: Use of Safety and Emergency equipment:

1. First aid Kits
2. Sand bucket
3. Fire extinguishers (dry chemical and carbon dioxide extinguishers)
4. Chemical Storage cabinet with proper ventilation
5. Material Safety Data sheets.
6. Management of Local exhaust systems and fume hoods.
7. Sign in register if using instruments.

M. Sc. Part – I (Semester – I)
Paper MCT-101: Inorganic Chemistry

Learning objectives:

1) To introduce students with chemistry of transition elements
2) To introduce students with different organometallic compounds and their chemistry
3) Students should know the metal-ligand equilibrium
4) Students should know the nanoscience and nanomaterials

Unit-I: Chemistry of transition elements [15]

General characteristic and properties of transition elements, Coordination chemistry of transition metal ions, Stereochemistry of coordination compounds, Crystal field theory for tetrahedral, octahedral, square pyramidal and square planar complexes, Splitting of dorbital's, Crystal field stabilization energy (CFSE), Factors affecting the crystal field parameters, Spectrochemical series, Jahn-Teller effect, Interpretation of electronic spectra including d-d and charge transfer spectra.

Unit II Organometallic Chemistry [15]

Synthesis, bonding in pi-metal organometallic complex, structure and reactivity of organometallic compounds, Classification of organometallic compounds based on hapticity and polarity of M-C bond, Nomenclature and general characters, 18 electron rule-applications and exceptions, Reactions of organometallic compounds: Oxidative addition, reductive elimination, Insertion and elimination, Organometallics in homogeneous catalysis: Hydrogenation, hydroformylation, isomerization and polymerization

UNIT III: A) Metal-ligand Equilibrium in solution [08]

Thermodynamic vs. kinetic stability, Stability constant, Stepwise and overall stability constants with their relation, Trends in stepwise stability constant, Factors affecting the stability of metal complexes with reference to the nature of metal ion and ligand, Chelate effect, Determination of stability constants by spectrophotometric methods (Job's and Mole/slope ratio for composition), Bjerrum's pH metric method.

B] Transition metal carbonyls and related compounds [07]

Introduction, Preparation, structure, physical and chemical properties of metal carbonyls, Anionic and cationic carbonyl complexes, Lewis base derivatives of carbonyls, Carbonyl hydrides, Carbonyl halides.

UNIT IV: Nanoscience and Nanomaterials [15]

Introduction to nanoscience and nanotechnology; historical background; Classification of nanomaterials: 1D, 2D, 3D (with their examples); Applications of nanotechnology

&Nanomaterials; Implications of nanotechnology; Future fantasy and nanotechnology; Experimental methods for preparation of nanomaterials: Chemical and Physical; Size dependent properties of nanoparticles; Characterization techniques for nanomaterials: Principle instrumentation and applications of XRD, SEM and TEM

Recommended references

1. J. D. Lee, Concise Inorganic Chemistry, John Wiley & Sons, 5th edition, 2009
2. B. R. Puri, L. R. Sharma and K. C. Kalia, Principals of Inorganic Chemistry, 2007-2008.
3. D. F. Shriver and P. W. Atkins, Inorganic Chemistry, Oxford, 3rd edition, 1999.
4. L. E. Smart, E. A. Moore, Solid State Chemistry: An Introduction.
5. T. Pradeep, Nano The Essentials: Understanding Nanoscience and Nanotechnology.
6. J. H. Huheey, Inorganic Chemistry - Principles, structure and reactivity, Harper and Row Publisher, Inc. New York, 1972.
7. Manas Chanda, Atomic Structure and Chemical bonding,
8. M. N. Hughes, Inorganic Chemistry of Biological Processes,
9. F. A. Cotton, R. G. Wilkinson. Advanced Inorganic chemistry,
10. N. N. Greenwood and A. Earnshaw, Chemistry of elements, Pergamon,
11. B. N. Figgis and M. A. Hitachman, Ligand field theory and its application, (2000) Wiely VCH publication.
12. Martel, Coordination chemistry.
13. Jones, Elementary co-ordination chemistry.
14. S. J. Lippard, J. M .Berg, Principles of bioinorganic Chemistry, University Science books.
15. R. J. P. Williams and F. R. Desalnia, Biological chemistry of the elements.
16. A. F. Wells, Structural Inorganic Chemistry – 5th edition, 1984.
17. M. C. Day and J. Selbin, Theoretical Inorganic Chemistry, Reinhold, EWAP,
18. A. H. Hanney, Solid State Chemistry, A. H. Publications,
19. O. A. Phiops, Metals and Metabolism,
20. S. J. Lippard, J. M. Berg, Principles of bioinorganic Chemistry, University Science Books,
21. G. L. Eichhron, Inorganic Biochemistry, Vol I and II, Elesevier,
22. Progress in Inorganic chemistry, Vol 18 and 38, J. J. Loppard, Wiley,
23. G. Zhong Cao. Nanostructures and Nanomaterials: Synthesis, Properties and Applications, Imperial College Press (2004).
24. M. Ratner & D. Ratner. Nanotechnology: A Gentle Introduction to the Next Big Idea, Pearson Education (2003).

Learning outcomes

UNIT I: Chemistry of Transition Elements

Students gain basic idea and knowledge about

1) chemistry of transition elements for their coordination compounds.
2) different theories for coordination compounds.
3) role of ligands incoordination compounds.
4) applications of coordination compounds.

UNIT II: Organometallic Chemistry

1) Student must explain formation of coordination compound and molecules.
2) Student must know bonding in organometallic compounds.
3) Student should know catalytic reactions of organometallic compounds.

UNIT III: A] Metal-ligand Equilibrium in solution

1) Student should understand stability constants.
2) Student should understand the Chelate effect.
3) Student should know Determination of stability constants by spectrophotometric methods.

B) Transition metal carbonyls and related compounds

1) Student must know metal carbonyls and related compounds.
2) Student must know physical and chemical properties of metal carbonyls.
3) Student should know carbonyl complexes.

UNIT IV: Nanoscience and Nanomaterials

1) They must know nanoscience and nanotechnology.
2) They should explain applications of nanotechnology.
3) They should understand different nanomaterials.
4) They should know future fantasy of nanomaterials.
5) They should know experimental methods for synthesis of nanomaterials.
6) They should know characterization techniques and properties of nanomaterials.

Paper MCT-102: Organic Chemistry

Learning Objectives

1) Students can be able to know different reactive intermediate also concept of aromaticity
2) Students get knowledge regarding the mechanism of different types of substitution reactions.
3) They can be able to get knowledge regarding the mechanism and types of elimination reactions.
4) Students get the knowledge regarding the important basic concepts of the stereochemistry.

Unit-I: Reaction Mechanism: Structure and Reactivity (15)

Types of reactions, Chemical bonding and basis of reactivity- Chemical bond, delocalization, conjugation, resonance, hyper conjugation, tautomerism, inductive effects. **Acidity and basicity:** various structural effects, hard and soft acid and base concept.; **Aromaticity:** Structural, thermochemical, and magnetic criteria for aromaticity, including NMR characteristics of aromatic systems. Benzenoid and non-benzenoid compounds, Huckels rule, antiaromaticity, Application to carbocyclic and heterocyclic systems, nulenes, azulenes, tropylium cations, metallocenes , current concepts of aromaticity.; **Structure and stability of reactive intermediates**, carbenes, nitrenes, carbocations, carbanions and free radicals.

R1- 14-21, 68-72, 275
R2- 122-131, 148, 152

UNIT-II: A) Aliphatic Nucleophilic substitutions: (7)

The SN2, SN1 and SNi reactions with respects to mechanism and stereochemistry. Nucleophilic substitutions at an allylic, aliphatic trigonal, benzylic, aryl and vinylic carbons. Reactivity effect of substrate structure, effect of attacking nucleophiles, leaving groups and reaction medium. SN reactions at bridge head carbon, competition between SN1 andSN2, Ambident nucleophiles, Neighboring Group Participation.

B) Aromatic Electrophilic Substitutions (8)

Introduction, the arenium ion mechanism, orientation and reactivity in Nitration, Sulphonation, Friedel-Crafts and Halogenation in aromatic systems, energy profile diagrams. The ortho/para ratio, ipso attack, concept of aromaticity, orientation in their ring systems. Diazo-coupling, Vilsmeier reaction, Von Richter rearrangement.

R1- 130-167, 31-45, 77-102
R11 – 121-149, 255-277

UNIT-III: A] Addition reactions (7)

Addition to C-C multiple bonds - mechanism and stereochemical aspects of addition reaction involving electrophile, nucleophile and free radicals, Regio and chemoselectivity, orientation and reactivity, conjugate addition.

B)Elimination Reactions: (8)

The E1, E2 and E1cB mechanisms. Orientation in Elimination reactions. Hoffman Versus Saytzeff elimination, competition between substitution and elimination reactions, Reactivity: effects of substrate structures, attacking base, the leaving group, the nature of medium on elimination reactions. Pyrolytic elimination reactions. Pyrolytic elimination: Chugaev reaction, Cope reaction and Pyrolysis of acetates.

R1- 248- 260, 381, 268, 340
R2- 573-583, 672

R3 – 335,336,420,610

UNIT-IV Stereochemistry (15)

Introduction:

Molecules with two or more chiral centers: Configurational nomenclature **Constitutionally unsymmetrical molecules:** Erythro-Threo and Syn-Anti systems. **Constitutionally symmetrical molecules with odd and even number of chiral centres:**

Enantiomeric and meso forms, concept of stereogenic, chirotopic and pseudo asymmetric centres.

Axial and planar chirality: Principles of axial and planar chirality. **Prochirality:** Homotopic, heterotopic and diastereotopic ligands and faces. Identification using substitution and symmetry criteria. Nomenclature of stereoheterotopic ligands and faces. Symbols for stereoheterotopic ligands in molecules with one or more prochiral centres, pro-pseudo asymmetric centre, chiral and prochiral centre; prochiral axis and prochiral plane. Symbols for enantiotopic and diastereotopic faces.

R7- 120-132, 325-367

R17- 30-72, 168-205

References:

1. A guide book to mechanism in Organic chemistry (Orient-Longmens)- 6th edition Peter Sykes
2. Organic Reaction Mechanism (Benjamin) R. Breslow
3. Organic Chemistry-7th edition R. T. Morrison and R. N. Boyd (Prentice Hall.)
4. Mechanism and Structure in Organic chemistry (Holt Reinh.) B. S.Gould.
5. Organic Chemistry (McGraw-Hill) Hendrikson, Cram and Hammond.
6. Reactive Intermediates in Organic Chemistry (John Wiley) N. S.Issacs.
7. Stereochemistry of Carbon Compounds. (McGraw-Hill)E. L. Eliel
8. Organic Stereochemistry (McGraw-Hill) by Hallas.
9. Organic Reaction Mechanism (McGraw-Hill) R. K. Bansal.
10. Basic principles of Organic Chemistry (Benjamin) J. D. Roberts and M. C. Caserio
11. Modern Organic Reactions (Benjumin) H. O. House.
12. Principle of organic synthesis- R.O.C. Norman and J. M. Coxon.(ELBS)
13. Reaction Mechanism in Organic Chemistry- S. M. Mukharji and S. P.Singh.
14. Stereochemistry of Organic compounds- D. Nasipuri.
15. Advanced Organic Chemistry (McGraw-Hill) J. March.
16. Introduction to Stereochemistry (Benjumin) K. Mislow.
17. Stereochemistry by P. S. Kalsi (New Age International)

Learning outcomes

Unit-I: Reaction Mechanism: Structure and Reactivity

1) Student should understand organic reaction mechanism with respect to structure and reactivity.
2) Student must explore conceptual fact of Chemical bonding and basis of reactivity.
3) Understanding formation of atomic orbital through quantum approach.
4) They should know energy level in atom using modern classical quantum mechanics.
5) They should understand behavior of electron in atom.

UNIT-II: A) Aliphatic Nucleophilic substitutions and B) Aromatic Electrophilic Substitutions

1) Student should understand formation of various types of Aliphatic Nucleophilic substitutions.
2) Student should compare The SN2, SN1 and SNi reactions with respects to mechanism and stereochemistry.
3) Student should know Ambident nucleophiles, Neighbouring Group Participation.
4) Student must explain Aromatic Electrophilic Substitutions.
5) Student must state approach of the arenium ion mechanism, orientation and reactivity in Nitration, Sulphonation, Friedel-Crafts and Halogenation in aromatic systems.
6) They should demonstrate concept of aromaticity, orientation in their ring systems. Diazo-coupling, Vilsmeier reaction, Von Richter rearrangement.

UNIT-III: A] Addition reactions and B) Elimination Reactions

1) They must explain the Addition to C-C multiple bonds - mechanism and stereochemical aspects of addition reaction.
2) They should explain nucleophile and free radicals, Regio and chemoselectivity,
1) They should understand Regio and chemoselectivity, orientation and reactivity, conjugate addition
2) Student must explain E1, E2 and E1cB mechanisms. Orientation in Elimination reactions
3) Student must state approach of the Hofman versus Saytzeff elimination
4) They should demonstrate concept of Pyrolytic elimination: Chugaev reaction, Cope reaction and Pyrolysis of acetates.

UNIT-IV: Stereochemistry

1) Student should understand configurations of molecules with two or more chiral centers
2) Student should understand Constitutionally symmetrical and unsymmetrical molecules.
3) Student should know Homotopic, heterotopic and diastereotopic ligands and faces.

Paper –MCT-103: Physical Chemistry

Course objective: Students should

1) Understand the application Gibbs- Duhem equation to study partial quantities.
2) Learn the theoretical Statistical Thermodynamics.
3)Learn the study of macromolecules chemistry.
4) study the basic concepts of Molecular Spectroscopy

UNIT-I:Thermodynamics [15]

Introduction, revision of basic concepts: Entropy and third law of thermodynamics. Methods of determining the practical absolute entropies. Entropies of phase transition. Maxwell relations and its applications, thermodynamic equation of state. Ideal and non-ideal solutions, Thermodynamics of nonelectrolyte solutions. Raoult's law. Duhem-Margules equation and its applications to vapor pressure curves (Binary liquid mixture). Gibbs-Duhem equation and its applications to study of partial molar quantities. Chemical potential, variation of chemical potential with temperature & pressure. Henry's law. Excess and mixing thermodynamic properties. Equilibrium constants and general conditions of equilibrium in terms of thermodynamic potentials. Numerical Problems.

R1. : Page No:28-105

UNIT-II: Statistical Thermodynamics [15]

Probability and distribution, Stirling Approximation, Weights and configurations, the most probable configuration, Ensembles, ensemble average and time average of property. Statistical equilibrium, thermodynamic probability, Maxwell-Boltzmann (MB) distribution law. Partition function and its significance. Rotational, translational, vibrational and electronic partition functions. Relationship between partition function and thermodynamic properties. thermodynamic probability and entropy: Boltzmann – Planck equation, Partition function and third law of thermodynamics, Application to monoatomic gases - Sackur tetrode equation, applications to diatomic molecules, Statistical expression for equilibrium constant, Limitations of Maxwell-Boltzmann statistics, Numerical Problems.

R1 : Page No: 560-620;
R7: entire book
R10:entire book

UNIT-III: Macromolecules[15]

Macromolecules: Mechanism of polymerization, molecular weight of a polymer (Number and mass average) viscosity average molecular weight, numerical problems. Degree of polymerization and molecular weight, practical significance of polymer molecular weight, methods of determining molecular weights (Osmometry, viscometry, light scattering, diffusion and ultra centrifugation)

Chemistry of polymerization: Ceiling temperature, Free radical polymerization (Initiation, propagation and termination), kinetics of free radical polymerization, step growth polymerization (Polycondensation), molecular weight distribution, kinetics of step polymerization, cationic and anionic polymerization. Electronically conducting polymers, thermodynamics of polymer solutions: Flory-Huggins Theory. Glass transition temperature and molecular weight, factors influencing Glass transition temperature, determination of glass transition temperature

R13:.Entire book
R17: Entire book
R18. Entire book

UNIT- IV: Molecular Spectroscopy [15]

Recapitulation: Width and intensity of spectral transitions, Fourier transform, Signal-to-noise ratio, Microwave spectroscopy, rotation spectra of diatomic molecules-rigid and non-rigid molecules, Stark effect. Infra- red spectroscopy: Harmonic and anharmonic oscillator, types of vibrational spectra of diatomic molecules, application Electronic spectroscopy of molecules: Born – Oppenheimer approximation, electronic spectra of diatomic molecules, application.

R1: 481-557
R16. : Relevant pages

References

1. Physical Chemistry – P. W. Atkins, Oxford University press, 8th edition,2006.
2. Text book of Physical Chemistry – S. Glasstone.
3. Principles of Physical Chemistry – Marron and Pruton.
4. Physical Chemistry – G. M. Barrow, Tata-McGraw Hill, Vth edition,2003.
5. Thermodynamics for Chemists – S. Glasstone, D. Van Nostrand ,1965.
6. Thermodynamics: A Core Course- R. C. Srivastava, S. K. Saha and A. K. Jain, Prentice-Hall of India, II nd edition,2004.
7. Elements of statistical thermodynamics - L. K. Nash, 2nd Ed. Addison Wesley 1974.
8. Theoretical Chemistry: An introduction to quantum mechanics, statistical mechanics, and molecular spectra for chemists - S. Glasstone, D. Van Nostrand Company, Inc.,1944.
9. An Introduction to Statistical Thermodynamics – T.L. Hill, Addison-Wesley. 1960.
10. Statistical Mechanics – Donald A. McQuarrie,2000.

11. Physical chemistry of surfaces – A. W. Adamson, 4th Ed. John Wiley,1982.
12. Introduction to Colloid and Surface Chemistry – D. Shaw, Butterworth Heinemann, 1992.
13. Surface Activity: Principles, Phenomena and Applications (Polymers, Interfaces and Biomaterials) – K. Tsujii, 1st Ed. Academic Press,1998.
14. Thermodynamics of Biochemical Reactions – R.A. Alberty, Wiley- Interscience, 2003.
15. Textbook of Biophysical Chemistry – U.N. Dash, McMillan India,2006.
16. Fundamentals of molecular spectroscopy : C.N. Banewell and E.Mc. Cash (Fourth edition).
17. *Physical Chemistry of macromolecules- D. D. Deshpande, Vishal Publications.*
18. *Polymer Chemistry- F. W. Billmeyer Jr, John-Wiley & Sons, 1971.*

Learning outcomes

UNIT-I: Thermodynamics

1) Student will understand difference between classical thermodynamics and modern thermodynamics
2) Student must explore applications of ideal solution and non-ideal solutions.
3) Understanding entropy and its application.
4) They will know equilibrium and equilibrium constants.
5) They will able to understand Maxwell relations.

UNIT-II: Statistical Thermodynamics

1) Student will able to compare formation of ensembles.
2) Student will know formation and energetics of Rotational, translational, vibrational and electronic partition functions.
3) They can explain Boltzmann – Planck equation. Ensembles, ensemble average and time average of property
4) Student must explain Sackur-tetrode equation.

UNIT-III: Macromolecules

1) Student will able to explain mechanism of polymerization, molecular weight of a polymer viscosity average molecular weight
2) Students will able to understand chemistry of polymerization: Ceiling temperature, Free radical polymerization, step growth polymerization (Polycondensation),cationic and anionic polymerization
3) Students will understand thermodynamics of polymer solutions: Flory-Huggins Theory. Glass transition temperature, determination of glass transition temperature

UNIT- IV: Molecular Spectroscopy

1) They must explain the Microwave spectroscopy, rotation spectra of diatomic molecules-rigid and non-rigid molecules

2) They should explain Infra- red spectroscopy, Harmonic and anharmonic oscillator, types of vibrational spectra of diatomic molecules.
3) Electronic spectroscopy of molecules: Born – Oppenheimer approximation, electronic spectra of diatomic molecules

Paper MCT-104: Analytical Chemistry

Learning Objectives:

1. Students should know what is error and different types of errors.
2. They also understand importance of error minimization in any analysis.
3. Students should familiar with different types of chromatographic techniques.
4. Students understand fluorescence and phosphorescence with respect to analytical applications.
5. Students should know what is Thermal Analysis, TGA, DTA and DSC.

UNIT-II: Errors and treatment in Analytical Chemistry [15]

Errors, Determinant, constant and indeterminate. Accuracy and precision, Distribution of random errors. Average deviation and standard deviation, variance and confidence limit. Significance figures and computation rules. Least square method. Methods of sampling: samples size. Techniques of sampling of gases, fluid, solids, and particulates.

UNIT-II: Chromatographic methods [15]

General principle, classification of chromatographic methods. Nature of partition forces. Chromatographic behavior of solutes. Column efficiency and resolution. Gas Chromatography: detector, optimization of experimental conditions. Ion exchanges chromatography. Thin layer chromatography: coating of materials, prepative TLC. Solvents used and methods of detection Column chromatography: Adsorption and partition methods. Nature of column materials.
Preparation of the column. Solvent systems and detection methods.

UNIT-III: Luminescence Spectrometry [15]

Introduction, Comparison of absorption and fluorescence methods, Theory, Instrumentation, applications of fluorimetry, Applications of Phosphometry, Comparison of Fluorimetry and Phosphometry.

UNIT-IV: Thermal Analysis [15]

Introduction to thermal analysis, types of thermal analysis, significance of thermal analysis in Analytical Chemistry, effect of heat on materials, chemical decomposition,

phase transformation etc. and general thermal analysis applications, advantages and disadvantages.

A) Thermo gravimetry analysis (TGA),

Principle, instrumentation, working, types of TGA, factors influencing TGA, curve to show nature of decomposition reactions, the product and qualities of compounds expelled, TGA in controlled atmosphere, TGA curves, analysis, research and analytical implications of TGA.

B) **Differential thermal analysis (DTA),**

Instrumentation, methodology, application and research implications. Thermometric titrations method and applications Problems: Simple problems based on TGA, DTA and DSC.

C) **Differential scanning calorimetry (DSC)**

Instrumentation, methodology, application and research implications. Thermometric titrations method and applications Problems: Simple problems based on TGA, DTA and DSC.

References:

1. Analytical Chemistry: (J.W) G. D. Christain
2. Introduction to chromatography: Bobbit
3. Instrumental Methods of analysis (CBS)- H.H . Willard, L.L. Mirrit, J. A. Dean
4. Instrumental Methods of Analysis :Chatwal and Anand
5. Instrumental Methods of Inorganic Analysis(ELBS) : A. I. Vogel
6. Chemical Instrumentation: A Systematic approch- H. A. Strobel
7. The principals of ion-selective electrodes and membrane transport: W.E. Morf
8. Physical Chemistry –P. W. Atkins
9. Principal of Instrumental Analysis- D. Skoog and D. West
10. Treatise on Analytical Chemistry: Vol Ito VII – I.M. Kolthoff
11. Computer, Fundamentals-P. K. Sinha
12. Programming in BASIC : E. Balaguruswamy
13. Computer programming made simples:J.Maynard.
14. Instrumental methods of chemical analysis-H.K.Kaur
15. Instrumental methods of chemical analysis-Chatwal and Anand
16. Instrumental methods of chemical analysis-B.K.Sharm.

Learning Outcomes

UNIT-I: Errors and treatment in Analytical Chemistry

1) Student should understand Errors, Determinant, constant and indeterminate. Accuracy and precision Distribution of random errors.
2) Student must explore conceptual fact of Average derivation and standard derivation, variance and confidence limit. Significance figures and computation

rules.

3) Student should understand Least square method. Methods of sampling: samples size.

UNIT-II: Chromatographic methods

1) Student should understand General principle, classification of chromatographic methods. Nature of partition forces. Chromatographic behavior of solutes.
2) Student should know Column efficiency and resolution. Gas Chromatography: detector, optimization of experimental conditions. Ion exchanges chromatography.
3) Student must know the Solvent systems and detection methods.

UNIT-III: Luminescence Spectrometry

1) Student must know Comparison of absorption and fluorescence methods.
2) Student must know Instrumentation, applications of fluorimetry.
3) Student should know Comparison of Fluorimetry and Phosphometry.

UNIT-IV: Thermal Analysis

1) Student should understand General principle, classification of Thermal Analysis.
2) Student must know Instrumentation, applications of Thermo gravimetry analysis (TGA) and Differential thermal analysis (DTA)
3) Student should know Comparison of Thermo gravimetry analysis and Differential thermal analysis.

MCP-105 : Lab I : Chemistry Practical -I

Learning objective: Students should

1) Learn ore , alloy analysis
2) Study preparation of coordination complexes.
3) Learn instrumentation techniques.
4) Learn single stage preparation by of important Organic products
5) Learn estimation of dyes, formalin and amino acids.

A) Inorganic Chemistry

A) Ore Analysis

Determination of Silica and Manganese in pyrolusite

Determination of iron from hematite.

B) Alloy Analysis

Determination of tin & lead from solder

Determination of copper and nickel from monel metal

C) Preparations and purity (Any four)

Potassimtrioxalatochromate(III) trihydrate
cis-potassium dioxalatodiaquachromate(III)
Potassionhexathiocyanatochromate(III)
Bis(dimethylglyoximato)nickel(II)
Carbonatotetramminocobalt(III) nitrate
Hexamminocobaltic(III) chloride

D) Determination of concentration of phosphates in water samples colorimetrically

Any other suitable experiment may be added.

Reference:

1. A text book of Quantitative Inorganic Analysis – A. I. Vogel
2. Experimental Inorganic Chemistry - W. G. Palmer
3. The analysis of minerals and ores of the rarer elements – W. R. Schoeller and A.R. Powell, Charles, Griffin and Company Limited
4. I. M. Kolthoff, V. J. Elving and Sandell, "Treatise on Analytical Chemistry", Interscience.
5. I. M. Kothoff and Strenger, "Volumetric Analysis",Interscience
6. Fruman and Welcher, "Standard Methods of Inorganic Analysis", VanNostrand
7. G. Schwarzenback, "Complexomtric Titrations",Interscience
8. D. A. Skoog and D.M. West, "Analytical Chemistry – An Introduction",Reinholdt.
9. R.S. Drago, "Physical Methods in Inorganic Chemistry", Affiliated East-West Press

Learning Outcomes

1) Student should understand the practical's of Inorganic Chemistry.
2) Student must explore different ore and alloy analysis of different metal compositions.
3) Student should understand preparations and purity of inorganic chemistry.

B) Organic Chemistry

A) Preparations

(One stage preparations involving various types of reactions)

1.Oxidation: Adipic acid by chromic acid oxidation of Cyclohexanol.

2.Aldol condensation: Dibenzaloacetone from Benzaldehyde.

3.Sandmeyer reaction: p- Chlorotoulene from p-Toluidine.

4.Cannizzaro reaction: 4- chlorobenzyldehyde as a substrate.

5.Aromatic Electrophilic substitutions: Synthesis of p-Nitroaniline and p-Bromoaniline.

6.Preparation of Cinnamic acid by Perkin's reaction.

7.Knoevenagel condensation reaction

8.Coumarin Synthesis

9.Synthesis of Heterocyclic compounds.

10. Synthesis of Dyes

11. Determination of percentage of Keto-enol form.

B) Estimations:

12.Estimation of formalin.

13.Colorimetric Estimation of Dyes

14.Estimation of Amino acids

(Any suitable Expt. may be added.)

References:

1.A text book of practical organic chemistry- A. I. Vogel.

2.Practical organic chemistry- Mann and Saunders.

3.Handbook of quantitative and qualitative analysis- H. T. Clarke.

4.Organic Synthesis Collective Volumes by Blat.

Learning outcomes

1) Student should understand variety of applications of name reactions.
2) Student should know the estimations and preparations of organic compounds.
3) Student should learn number of organic synthesis.

MCP-106: Lab-II: Chemistry Practical –II

Course Objective: Students should

1) Study potentiometric analysis
2) study the handling of instrumentations
3) Learn rate of reactions, kinetics of reactions
4)Learn the analysis of pharmaceutical tablets..
5) Study estimation of Ca, Na, chloride, bromide ions.

A) Physical Chemistry

Students are expected to perform 15-20 experiments of three and half hours duration.

Experiments are to be set up in the following techniques.

1. Potentiometry:

i)Determination of solubility and solubility product of silver halides.

ii) Determination of binary mixture of weak and strong acid.

2. Conductometry:

i) Determination of mixture of acids and relative strength of weak acids.

ii) Hydrolysis of ethyl acetate by NaOH using conductometric measurements.
iii) Determination of ΔG, ΔH, and ΔS of $BaSO_4$ by conductometry.

3.Spectrophotometry:

To Study the kinetics of iodination of acetone spectrophotometrically.

4.Refractometry :

Determination of molecular radius of molecule of organic compound.

5.Polarimetry :

Kinetics of inversion of cane sugar in presence of strong acid.

6.Chemical Kinetics:

Kinetics of reaction between bromate and iodide.

7.Partial Molar Volume:

Determination of PMV by intercept method, density measurements etc.

(New experiments may also be added)

References:

1 Findlay's Practical Chemistry – Revised by J.A. Kitchner (V edition)
2 Text Book of Quantitative inorganic analysis : A.I. Vogel.21
3 Experimental Physical Chemistry :R.C. Das and B. Behera
4 Practical Physical Chemistry : B. Viswanathan and P.S. Raghavan
5 Experimental Physical Chemistry :V.D. Athawale and Parul Mathur.
6 Systematic Experimental Physical Chemistry :S.W. Rajbhoj and T.K. Chondhekar

Learning outcomes

1) Student should understand variety of instrumentation techniques..
2) Student should know the spectrophotometric experiments.
3) Student should learn chemical kinetics of the reaction.

B. Analytical chemistry

i) Physical Chemistry Section

1) To verify Beer-Lambert's Law for potassium permanganate solution and hence To determine the molar extinction coefficient and unknown concentration of given sample colorimetrically
2) To determine the solubility of calcium oxalate in presence of KCl (Ionic strength Effect)
3) To determine the solubility of calciuum oxalate in presence of HCl (H^+ ion Effect)

ii) Organic Chemistry Section

1 Analysis of Pharmaceutical tablets.
2 To verify the Beer-Lamberts Law and determine the concentration of given dye solution colorimetrically.
3 To estimate the amount of D-glucose in given solution colorimetrically.

4 To determine the acid value of given oil.

iii) Inorganic Chemistry Section

1 Determination of sodium from the fertilizer sample using cation exchange chromatographically.

2 Determination of calcium from given drug sample.

3 Determination of hardness, alkalinity and salinity of water sample

4 Separation and estimation of chloride and bromide on anion exchanger.

References:

1 A Text book of quantitative Inorganic Analysis – A.I. Vogel

2 Standards methods of Chemical Analysis-F.J. Welcher.

1.Experimental Inorganic Chemistry –W.G. Palmer.

2. Manual on Water and Waste Water Analysis, NEERI- Nagpur D.S. Ramteke and C.A.Moghe

3.Inorganic synthesis-King.

4.Synthetic Inorganic Chemistry- W.L.Jolly 7 EDTA Titrations–F.Laschka

Learning Outcomes

1) Student should understand the practical's of Physical, Inorganic and Organic Chemistry with respect to analytical Chemistry.
2) Student must explore different concepts of practicals in three different disciplines of chemistry.
3) Student should understand applications of experimental chemistry through analytical chemistry.

M. Sc. Part – I (Semester – II)

Paper MCT-201: Inorganic Chemistry

Learning objectives:

1) To introduce students with chemistry of non-transition elements
2) To introduce students with stereochemistry and bonding in main group compounds
3) Students should know the chemistry of f-block elements
4) Students should know the Group Theory and Molecular Symmetry

UNIT I: Chemistry of Non-transition Elements and their compounds [15]

General discussion on the properties of the non–transition elements, Polymorphism in carbon, phosphorous and sulphur, Synthesis, properties and structure of boranes, carboranes, silicates, phosphazenes, sulphur–nitrogen compounds, peroxo compounds of

boron, carbon, sulphur, structure and bonding in oxyacids of nitrogen, phosphorous, sulphur and halogens, interhalogens, psudohalides.

UNIT II: A) Stereochemistry and bonding in Main group compounds [08]

Hybridization and structure of molecules, VSEPR Theory, pπ-pπ and pπ-dπ bonds, Bent rule, Walsh Diagram, Back bonding, Some simple reactions of covalently bonded molecules (atomic inversion, Berry Pseudorotation, Nucleophilic displacement, free radical reaction)

B) Bioinorganic Chemistry [07]

Role of metal ions in biological processes, structure and properties of metalloproteins, porphyrines, cytochromes, ferrodoxins and iron sulphur proteins, ion transport across membranes, Nitrogen fixation nitrogenase.

UNIT III: Chemistry of f-block elements (Lanthanides and Actinides) [15]

Occurrence, properties of the f-block elements, colour, oxidation state, Spectral and magnetic properties of lanthanides and actinides, lanthanide contraction, Use of lanthanide compounds as shift reagents, compounds of lanthanides, Photoluminescence properties of lanthanide compounds, Modern methods of separation of lanthanides and actinides, Applications of lanthanide and actinide compounds in Industries

UNIT IV: Group Theory and Molecular Symmetry [15]

Symmetry operations, Symmetry elements, Point group and its classification (Cn-type, Dn-type, Special-type), Schoenflies symbol for point groups, Determination of point group for AB_2(Bent), AB_3 (Trigonal pyramid), AB_3 (Trigonal Planar), AB_4 (Square planar), AB_5(Trigonal bipyramidal), AB_6 (Octahedral), CO_2, HCl, CO, Symmetry and dipole moment of molecule, Symmetry and optical activity Group and its Properties, Group multiplication table, Reducible and Irreducible representations, Properties of Irreducible representation, Great orthogonally theorem (without proof) and its importance, Construction of character table for C_2v & C_3v point groups, Mulliken symbolism rules for irreducible representations & its illustrations, Direct product, Standard reduction formula.

References

1. J. D. Lee, Concise Inorganic Chemistry, John Wiley & Sons, 5th edition, 2009
2. B. R. Puri, L. R. Sharma and K. C. Kalia, Principals of Inorganic Chemistry, 2007-2008.
3. D. F. Shriver and P. W. Atkins, Inorganic Chemistry, Oxford, 3rd edition, 1999.
4. T. Pradeep, Nano The Essentials: Understanding Nanoscience and Nanotechnology.
5. J. Schulte, Nanotechnology: Global Strategies, Industry Trends and Applications.
6. Ligand field theory and its application, B. N. Figgis and M. A. Hitachman (2000) Wiely VCH publication.
7. R. L. Datta and Syamal, Elements of magneto chemistry, Second edition, East west press pvt ltd. 2007.

8. B. P. Level, Inorganic Electronic Spectroscopy, second edition 1984, Elsevier Science publisher New York.
9. A. F. Wells, Structural Inorganic Chemistry – 5th edition, 1984.
10. J. H. Huheey, Inorganic Chemistry - Principles, structure and reactivity, Harper and
11. Row Publisher, Inc. New York, 1972.
12. Jones, Elementary coordination chemistry
13. Manas Chanda, Atomic Structure and Chemical bonding,
14. F. A. Cotton, R. G. Wilkinson. Advanced Inorganic chemistry,
15. P. L. Pauson, Organometallic chemistry
16. H. S. Sisler Chemistry in non aqueous solvent, Reinhold Publisher corporation, USA.
17. G. Schmid, Nanotechnology, Volume 1: Principles and Fundamentals.
18. L. E. Smart, E. A. Moore, Solid State Chemistry: An Introduction.
19. C. Kittel, Introduction to solid state Physics.
20. F. A. Cotton, Chemical applications of Group Theory, Third ed, John Wiley &Sons, Canada,1990.
21. P. Kelly, Symmetry, Handout of CHEM201, Fall 2008.
22. E. Wiberg, N. Wiberg, A. F. Holleman, Inorganic Chemistry, Academic Press, 2001.
23. Chemical Applications of Group Theory, F.A. Cotton, 3rd Edition, John Wiley & Sons, Inc. 2003
24. R. Drago: Physical method in Inorganic Chemistry, DUSAP.
25. Ferraro Ziomeek, Introduction to Group theory, plenum
26. Hall: Group theory and symmetry in Chemistry MGLt
27. P.K. Bhattacharya: Group Theory & Its Chemical Applications

Learning outcomes

UNIT I: Chemistry of Non–Transition Elements

1) Student should understand chemistry of non-transition elements for their coordination compounds.
2) Student should understand properties of the non–transition elements, Special features of individual elements.
3) Student should know Polymorphism in carbon, phosphorous and sulphur, Synthesis, properties and structure of boranes, carboranes, silicates, carbides, phosphazenes.
4) Student must know bonding in oxyacids of nitrogen, phosphorous, sulphur and halogens, interhalogens, pseudohalides.

UNIT II: A] Stereochemistry and Bonding in Main Group Compounds

1) Student should understand difference between classical chemistry and modern chemistry.
2) Student must explore conceptual fact of atom and molecule, understanding formation of

atomic orbital and behaviour of electron in atom.
3) Student should understand different bond formation.
5) Student should know reactions of covalent molecules.

B] Bioinorganic Chemistry

1) Student should know role of elements in biological processes.
2) Student must know the metalloprotiens in body, transport process and biomogical nitrogen fixation process

UNIT III: Studies and Applications of Lanthanides and Actinides

1) They must explain Spectral and magnetic properties, Use of lanthanide compounds as shift reagents, Modern methods of separation of lanthanides and actinides.
2) They must know separation techniques of Lanthanides
3) They should explain Organometallic chemistry applications of lanthanide and actinide compounds in Industries.

UNIT IV: Group Theory and Molecular Symmetry

1) They must know Symmetry operations.
2) They should know point-group and its classification.
3) They should understand matrix representation of symmetry elements.
4) They should know Direct product and standard reduction formula.
5) They should understand Nebulisation Torch, Plasmsa, Instrumentation.

Paper-MCT-202: Organic Chemistry

Learning Objectives:

1) Students are able to get knowledge regarding various important name reactions.
2) Students are knowledgeable with the important oxidizing and reducing agents.
3) Students are able to get the knowledge of hydroboration concept and it's synthetic Applications.
4) Students are able to get the knowledge of important organometallic compounds.

UNIT-I: A) Study of following reactions: (12)

Mechanism of condensation reaction involving enolates Mannich, Benzoin, Stobbe, Dieckmann, Robinson annulation, Chichibabin, Simon-Smith, Vlhmann, Mc-Murry, Dakin, Hoffman, Schmidt, Curtius, Lossen, Demjanov reaction and Suzuki coupling reaction.

B) Alkylation and Acylation (03)

Introduction, Types of alkylation and alkylating agents: C-Alkylation and Acylation of active methylene compounds and their applications.

R1- Entire book

R2- 1541, 816, 901, 325, 725-746

R3- 111-115, 169-172

UNIT-II:A)Oxidation (08)

CrO_3, PDC, PCC, $KMnO_4$, MnO_2, Swern, SeO_2, $Pb(OAc)_4$,Pd-C, OSO_4, m-CPBA, O_3, $NaIO_4$, HIO_4, RuO_4, Etard oxidation, H_2O_2 and Peracid.

B)Reduction (07)

General mechanism, selectivity, and important applications of the following reducing reagents: Metal hydride reduction: Boron reagents ($NaBH_4$, $NaCNBH_3$, $Na(OAc)_3BH$), Aluminium reagents ($LiAlH_4$, DIBALH, Red Al),reduction with H_2/Pd-C, Wilkinson's catalyst and Wolff Kishner reduction.

R 1- 89-112, 151-167, 226-239

R2- 503, 1472-1487, 563-576, 489-497

R-3- 575-605

UNIT-III: A)Hydroboration: (05)

Various hydroborating agents their Mechanism and Synthetic Applications viz 9- BBN, thexyl borane, diisamyl borane

B) Enamins: (05)

Formation and reactivity of enamines

C) Ylides: (05)

Phosphorus, Nitrogen and Sulphur ylides

R2- 1278-1283, 615-667,1275-1279, 1325-1339

R4- Entire book

UNIT-IV: Study of Organometallic compounds: (15)

Organo-lithium, organo cobalt, Fe, Ce, Ti, Cd. Use of lithium dialkyl cuprate,their addition to carbonyl and unsaturated carbonyl compounds.

R2- 771-798, 209-223, 1251-1258

R3- 15-52

References:

1. A collection of detailed reaction mechanism-2nd edition- Jie Jack Li

2. Organic Chemistry- 1st edition- Clayden, Greeves, Warren and Wothers
3. Some modern methods of Organic synthesis-(Cambridge) W. Carruthares.
4.Hydroboration- S. C. Brown.
5.Advances in Organometallic Chemistry- (A.P.)F. C. A. Stone and R. West.
6.Organic Chemistry (Longman)Vol. I & Vol. II- Finar
7. Oxidation by-(Marcel Dekker)Augustin
8.Advanced Organic chemistry 2nd Ed. R R. Carey and R. J. Sundburg.
9.Tetrahydron reports in organic chemistry- Vol.1, No.8.
10.Organic Synthesis-(Prentice Hall)R. E. Ireland.
11.Homogeneous Hydrogenation-(J. K.) B. R. James.
12.Comprehensive Organic Chemistry- (Pargamon) Barton and Ollis.
13.Organic reactions- various volumes- R. Adams.
14. Principles of organic synthesis-(Methuen) R. O. C. Norman
15. Modern synthetic reactions-(Benjamin) H. O. House.
16. Reagents in organic synthesis-(John Wiley) Fieser and Fieser

Learning outcomes

UNIT-I: A) Study of following reactions and B) Alkylation and Acylation

1) Student should understand organic reaction mechanism with respect to Mechanism of condensation reaction involving enolates Mannich, Benzoin, Stobbe, Dieckmann, Robinson annulation
2) Student must know the reaction Chichibabin, , Simon-Smith, Vlhmann, Mc-Murry, Dakin, Hoffman, Schmidt, Curtius, Lossen, Neberl and Prins, Ortaon, Hofmann-Martius and Demjanov reaction, Suzuki coupling reaction
3) Student must understand the Types of alkylation and alkylating agents: C-Alkylation and Acylation of active methylene compounds and their applications.

UNIT-II: A) Oxidation and B) Reduction

1) Student should explain mechanism of the reagents CrO_3, PDC, PCC, $KMnO_4$, MnO_2, Swern, SeO_2, $Pb(OAc)_4$,Pd-C, OSO_4, m-CPBA, O_3, $NaIO_4$, HIO_4, RuO_4, Etard
oxidation, H_2O_2 and Peracid.
2) They should understand its role in organic synthesis.
3) They must explain General mechanism, selectivity, and important applications of the following reducing reagents: Metal hydride reduction: Boron reagents ($NaBH_4$, $NaCNBH_3$, $Na(OAc)_3BH$), Aluminium reagents ($LiAlH_4$, DIBALH, Red Al), MPV reduction.

UNIT-III: A) Hydroboration, B) Enamins and C) Ylides

1) They must explain the Mechanism and Synthetic Applications of hydroboration.
2) They must explain the formation and reactivity of enamines.

3) Students should understand the chemistry of Nitrogen and sulpher with respect to their ylides.

UNIT-IV: Study of Organometallic compounds

1) Student should explain the reaction and mechanism of Organo-lithium, organo cobalt, Fe, Ce, Ti, Cd.
2) They must understand applications of organometallic compounds in organic synthesis.

Paper-MCT-203: Physical Chemistry

Course Objectives: Students should

1) understand the various Operators and Schrodinger equation.
2) study the photochemistry and fluorescence.
3) Learn the theroretical Huckel theory of inter- ionic attraction.
4) Study Homegeneous and Heterogeneous catalysis.

UNIT-I: Quantum Chemistry [15]

Introduction: Wave particle duality of material and De Broglie's hypothesis, uncertainty principle, Schrodinger equation, wave function, conditions for acceptable wave functions and its interpretation, properties of wave functions, Operators and related theorem, algebra of operators, commutator, linear operators, Normalization and orthogonality, Eigen functions and Eigen values, postulate of quantum mechanics. Solutions of wave equation for a free particle and particle in a box problem, Transition dipole moment integral and selection rules, particle in abox application to electronic spectra of conjugated linear organic molecules. Linear and angular momentum operators, eigenfunction and eigen values of angular momentum operator, Ladder operator, addition of angular momenta. Spin angular momenta, symmetric and antisymmetric wavefunctions, Pauli Exclusion Principle, spectroscopic term symbols.

R3: entire book
R7 : Page No.1- 100, 120-150 ;
R22: Page No.21-110, 111-172.

UNIT-II: A] Photochemistry [08]

Absorption of light and nature of electronic spectra, electronic transition, Frank Condon principle,selectionrules,photo-dissociation,pre-dissociation,Photo physical phenomena: Electronic structure of molecules, molecular orbital, electronically

excited singlet states, designation based on multiplicity rule, life time of electronically excited state, construction of Jablonski diagram, electronic transitions and intensity of absorption bands, photo-physical pathways of excited molecular system(radiative and nonradiative),Photochemistry of environment: Greenhouse Effect.

B] Fluorescence [07]

Introduction, delayed fluorescence, and phosphorescence, fluorescence quenching: concentration quenching, quenching by excimer and exciplex emission, fluorescence resonance energy transfer between photo-excited donor and acceptor systems. Stern-Volmer relation, critical energy transfer distances, energy transfer efficiency, examples and analytical significance, bimolecular collisional quenching and Stern-Volmer equation.

R9 : Relative pages
R10: Relative pages
R22: Page No.1112-1146

UNIT-III: Electrochemistry [15]

Debye - Huckel theory of inter-ionic attraction, ionic atmosphere, time of relaxation, relaxation and electro-phoretic effects, Debye-Huckel-Onsagar equation andits validity for dilute solutions and at appreciably concentrated solutions. Abnormal ionic conductance of hydroxyl and hydrogen ions. Activity coefficients: forms of activity coefficients and their interrelationship. Debye-Huckel limiting law for osmotic and activity coefficients of dilute electrolytic solutions and its applications to concentrated solutions. Debye-Huckel-Bronsted equations. Quantitative and qualitative verification of Debye-Huckel limiting law, Bjerrum theory of ion-ion association. Types of electrode, Determination of activity coefficients of an electrolyte using concentration cells, degree of dissociation of monobasic weak acid (approximate and accurate), instability constant of silver ammonia complex. Acid and alkaline storage batteries.

R18: Relevant pages
R22: 835- 881, 882-934

UNIT-IV: A]Chemical Kinetics [15]

Experimental methods of following kinetics of a reaction, chemical and physical(measurement of pressure, volume, EMF, conductance, diffusion current and absorbance)methods and examples. Steady state approximation and study of reaction between $NO_2$and F_2, decomposition of ozone, and nitrogen pentoxide. Ionic reaction: Primary and secondary salt effect, Homogeneous catalysis: acid and base catalysed reactions, Michaelis–Menten enzyme catalysis. Heterogeneous catalysis: Adsorption of gas on a surface and its kinetics, Catalyzed hydrogen-deuterium exchange reaction.

R16: 20-80, 100-180

R22: 1033- 1111

References:

1. Introductory Quantum Chemistry - A. K. Chandra. Tata McGraw-Hill.1988.
2. Physical Chemistry: A molecular Approach – Donald A. McQuarrie and John D. Simon, Viva Books, New Delhi, 1998.
3. Quantum Chemistry – Donald A. McQuarrie, Viva Books, New Delhi,2003.
4. Physical Chemistry – P. W. Atkins, Oxford University press, VIth edition,1998.
5. Quantum Chemistry - W. Kauzmann, Academic press.
6. Theoretical Chemistry: An introduction to quantum mechanics, statistical mechanics, and molecular spectra for chemists - S. Glasstone, D. Van Nostrand Company, Inc., 1944.
7. Quantum Chemistry - R.K. Prasad, New Age International, New Delhi.
8. Physical Chemistry – R.S. Berry, S.A. Rice, J. Ross, 2nd Ed., Oxford University Press, New York,2000.
9. Photochemistry – J. G. Calverts and J. N. Pitts, John-Wiley &Sons
10. Fundamentals of Photochemistry- K. K. Rohatgi-Mukharjii, Wiley Eastern
11. Introduction to Photochemistry-Wells27
12. Photochemistry of solutions-C. A. Parker, Elsevier
13. An Introduction to Electrochemistry by S. Glasstone
14. Modern Electrochemistry Vol. I & II by J. O. M. Bockris and A.K.N. Reddy.
15. Electrolytic Solutions by R. A. Robinson and R. H. Strokes,1959
16. Chemical Kinetics-K. J. Laidler, PearsonEducation,2004
17. Kinetics and Mechanism - A. A. Frost and R. G.Pearson.
18. Electrochemistry- S. Glasstone, D. Van Nostrand ,1965
19. Advanced Physical Chemistry- Gurdeep Raj, Goel Publishing House
20. Basic chemical Kinetics- G. L. Agarwal, Tata-McGrawHill
21. Physical Chemistry – G. M. Barrow, Tata-McGraw Hill, Vth edition,2003.
22. The principles of physical Chemistry-Puri Sharma Patania 5th Edition

Learning Outcomes

UNIT- I: Quantum Chemistry

1) Student should understand difference between Operators and related theorems
2) Student must explore applications of commutator, linear operators, uncertainty principle.
3) Understanding Solutions of wave equation for a free particle and particle in a box problem
4) They should know Transition dipole moment integral and selection rules.
5) They should Linear and angular momentum, eigen function and eigen values of

angular momentum operator, Ladder operator, addition of angular momenta.

UNIT-II: A] Photochemistry

1) Student should know selection rules, photo-dissociation,pre-dissociation.
2) Student should know Electronic structure of molecules, molecular orbital, electronically excitedsinglet states, designation based on multiplicityrule.

B] Fluorescence

1)They should explain prompt fluorescence, delayed fluorescence, and Phosphorescence.
2)Fluorescence quenching: concentration quenching, quenching byexcimer Andexciplex emission

UNIT-III: Electrochemistry

1) Student must explain Debye - Huckel theory of inter-ionic attraction, ionic atmosphere, time of relaxation.
2) Student must state Debye-Huckel-Onsagar equation and its validity for dilute solutions and at appreciably concentratedsolutions.
3) They should demonstrate Debye-Huckel-Bronsted equations. Quantitative and qualitative verification of Debye-Huckel limiting law, Bjerrum theory of ion-ion association.

UNIT-IV: Chemical Kinetics

1) Student must explain Experimental methods of following kinetics of a reaction, chemical and physical(measurement of pressure, volume, EMF, conductance, diffusion current andabsorbance)methods.
2) Student must state Steady state approximation and study of reaction between NO_2andF_2, decomposition of ozone, and nitrogenpentoxide.
3) They should demonstrate Heterogeneous catalysis: Adsorption of gas on as surface and its kinetics, Catalyzed hydrogen-deuterium exchangereaction
4) Student must explain Colloids and surfaces: Stability and properties of colloids; isotherms and surfacearea; heterogeneouscatalysis.

Paper MCT-204: Analytical Chemistry

Learning Objectives:

1. Students should know what is difference between absorpotion and emission spectra.
2. They also understand importance terms used in various spectroscopic methodes.
3. Students should familiar with UV, IR, NMR and Mass techniques.
4. Students understand interoritation of IR, NMR and mass spectra.
5. Students should also familiar with Mossbauer and ESR Spectroscopy.
6. Students should know atomic apsortion and inductively coupled flame ionization

spectroscopy.

UNIT-I: A] Ultraviolet and visible spectrophotometry(UV-VIS) (08)

Introduction, Electronic transitions, Terms used in UV spectroscopy, Beer Lambert's law, molar absorption, molar extinction coefficient, types of recording spectra (solid, liquid), Solvent effect, Factors affecting on UV absorption band, calculation of absorption maxima of dienes, dienones and polyenes, applications.

B] Infrared Spectroscopy(IR) (07)

Introduction, instrumentation, Fundamental modes of vibrations, Fundamental group region, sampling technique, selection rules, types of bonds, absorption of common functional groups. Factors affecting frequencies, applications.

UNIT-II: A] Nuclear Magnetic Resonance (NMR): (08)

Introduction, Magnetic and non-magnetic nuclei, Elementary ideas of NMR Integration, Larmor frequency, absorption of radio frequency. Instrumentation (FT-NMR). Sample preparation, chemical shift, Factor affecting chemical effect, spin-spin coupling, coupling constant, Cosy, Nosy, DEPT, 19F, 1H, 13C, 31P, and 14N NMR.
First order coupling, applications to simple structural problems .

B] Mass spectroscopy (MS): (07)

Instrumentation, working of mass spectrometer (double beam). Formation of different types of ions, Mclafferty rearrangements, Nitrogen rule, C-13 rule, fragmentation of alkanes, alkyl aromatics, alcohols and ketones, simple applications, simple structural problems based on IR, UV , NMR and MS

UNIT-III: A) Mossbauer Spectroscopy (07)

Introduction, Principle, spectral parameters and spectral display, application of studies of bonding structures of Fe^{+2} and Fe^{+3} compounds including those of intermediate, spin and Sn^{+2} and Sn^{+4} compounds.

B) Electron Spin Resonance Spectroscopy(ESR) (08)

Introduction, ESR of d^1 and d^9transition metal ions in cubic and tetragonal ligand fields, evaluation of g values and metal hyperfine coupling constant.

UNIT-IV: A) Atomic Absorption and Flame Emission Spectroscopy (10)

Introduction, Principal, difference between AAS and FES, Advantages of AAS over FES, advantages and disadvantages of AAS. Instrumentation, Single and double beam AAS, detection limit and sensitivity, Interferences applications.

B) Inductively coupled Plasma Spectroscopy (5)

Introduction, Nebulisation Torch, Plasmsa, Instrumentation, Interferences, Applications.

References:

1. Carey and Sundberg. (Ed. III) , Part B – Adv. Organic Chemistry.
2. H.O. House , Synthetic Organic Chemistry.
3. Gould E.S., Mechanism and Structure in Organic Chemistry.
4. Norman R.O.C. Organic Chemistry.
5. J. March,(Ed IV), Adv Organic Chemistry.
6. Silversteine and Basser, Spectrometric Identification of Organic Compounds.
7. Kalsi, Organic Spectroscopy.
8. J. Bellamy, Infrared spectra of Complex molecules.
9. I Fleming, Organic Spectroscopy.
10. J. Clayden, N.Greeves *et. al* Organic Chemistry
11. Eliel, Stereochemistry.
12. D. Nashipuri, Stereochemistry of Organic Compounds
13. Pavia Spectroscopy of Organic Compounds
14. Vogel Practical Organic Chemistry
15. Instrumental Methods of analysis- Willard, Merrit, Dean and Settle.
16. Spectroscopic methods in organic chemistry- D.H. Williams and I. Fleming
17. Absorption spectroscopy of organic molecules- V.M. Parikh
18. A Text book of Qualitative Inorganic Analysis- A. I. Vogel
19. Physical Methods in Inorganic Chemistry (DWAP)- R. Drago
20. Fundamentals of Analytical Chemistry – D.A. Skoog and D.M. West (Holt Rinehart and Winston Inc)

Learning Outcomes

UNIT-I: A] Ultraviolet and visible spectrophotometry (UV-VIS) and B] Infrared Spectroscopy(IR)

1) Student should understand Electronic transitions, Terms used in UV spectroscopy, Beer Lambert's law.
2) Student must explore conceptual fact of Solvent effect, Factors affecting on UV absorption band.
3) Student should understand Fundamental modes of vibrations, Fundamental group region, sampling technique, selection rules, types of bonds, absorption of common functional groups.

UNIT-II: A] Nuclear Magnetic Resonance (NMR) and B] Mass spectroscopy (MS)

1) Student should understand Fundamental modes of vibrations, Fundamental group region, sampling technique, selection rules, types of bonds, absorption of common functional groups.
2) Student should know Principle, working of mass spectrometer (double beam). Formation of different types of ions, Mclafferty rearrangements, Nitrogen rule, C-13 rule, fragmentation.

3) Student must know the structural problems based on IR, UV , NMR and MS.

UNIT-III: Mossbauer and ESR Spectroscopy

1) Student must know spectral parameters and spectral display.
2) Student must know bonding structures of Fe^{+2} and Fe^{+3} compounds including those of intermediate.
3) Student should understand ESR of d1 and d9transition metal ions in cubic and tetragonal ligand fields.

UNIT-IV: A) Atomic Absorption Spectroscopy and B) Inductively coupled Plasma Spectroscopy

1) They must explain Principal, difference between AAS and FES.
2) They should explain Advantages of AAS over FES, advantages and disadvantages of AAS.
3) They should understand Nebulisation Torch, Plasmsa, Instrumentation.

MCP-205: Lab -III Chemistry Practical-III

Learning Objective: student should

1) Learn ore, alloy analysis
2) Study preparation of coordination complexes.
3) Learn instrumentation techniques.
4) Learn organic qualitative analysis by ether separation.
5) Learn estimation of pesticides.

A) Inorganic Chemistry

A) Ore Analysis
- Determination of calcium and magnesium from Dolomite
- Determination of copper and iron from chalcopyrite

B) Alloy Analysis
- Determination of copper and zinc from brass alloy
- Determination of iron & chromium from steel.

C) Preparations and purity (Any four)
- Tris(acetylacetonato)cobalt(III) trihydrate
- Pentaaquachlorochromium(III) chloride
- Hexathioureaplumbus(II) nitrate
- Bis(acetylacetonato)copper(II)
- Diaquabis(ethylediammine)copper(II) iodide
- Copper ferrite

D) Synthesis of nanomaterials of$CuS/PbS/CdS/CuO/ZnO/TiO_2$

Any other suitable experiment may be added.

Reference:

1. A text book of Quantitative Inorganic Analysis – A. I.Vogel

2. Experimental Inorganic Chemistry - W. G.Palmer
3. The analysis of minerals and ores of the rarer elements – W. R. Schoeller and A.R. Powell, Charles, Griffin and Company Limited
4. I.M. Kolthoff, V.J. Elving and Sandell, "Treatise on Analytical Chemistry",Interscience.
5. I.M. Kothoff and Strenger, "Volumetric Analysis",Interscience
6. Fruman and Welcher, "Standard Methods of Inorganic Analysis", Van Nostrand
7. G. Schwarzen back, "Complexomtric Titrations",Interscience
8. D.A. Skoog and D.M. West, "Analytical Chemistry – An Introduction",Reinholdt.
9. R.S. Drago, "Physical Methods in Inorganic Chemistry", Affiliated East-West Press

Learning Outcomes

1) Student should understand the practical's of Inorganic Chemistry.
2) Student must explore different ore and alloy analysis of different metal compositions.
3) Student should understand synthesis of nanomaterials.

B) Organic Chemistry

1. Qualitative analysis:

Separation and identification of the two component mixtures using Chemical and physical methods.

2. Steam distillation techniques.

3. Estimation of pesticides

(Any other suitable experiments may be added).

References:

1.A text book of practical organic chemistry- A. I. Vogel.

2.Practical organic chemistry- Mann and Saunders.

3.A handbook of quantitative and qualitative analysis- H. T. Clarke.

4.Organic Synthesis Collective Volumes by Blat.

Learning Outcomes

1) Student should understand the qualitative analysis of organic chemistry.
2) Student should understand steam distillation techniques.
3) Student must explore to estimations of pesticides.

MCP-206: Lab-IV : Chemistry Practical –IV

Learning Objectives : students should

1) Study Instrumental analysis.
2) Study the chemical kinetic of reactions.
3) Learn phase equilibrium.
4) viscosity of compounds and solutions.
5) Learn estimation of Cu, Ni, Fe .
6) study analysis of pharmaceutical tablets.

A) Physical Chemistry

Students are expected to perform 15-20 experiments of three and half-hours duration. Experiments are to be set up in the following techniques.

1. Potentiometery:

i) Determination formal redox potential of system(Fe^{2+},Fe^{3+})

ii)Determination of binary mixture of halides.

iii) Determination of stability Constant of a silver ammonium complex.

2. Conductometry :

i) Titration of ternary acid mixture of acids.

ii) Verification of Onsagar Equation for 1:1 type strong electrolyte.

3 .Refractometry:

Determination of atomic refractions of H, C and Cl atoms.

4.Chemical kinetics:

Kinetics of iodination of acetone in presence of strong acid.

5.Phase Equilibrium:

To construct phase diagrams for ternary system.

6.Viscometry:

Determination of radius of glycerol molecule by viscosity.

7. To draw polar plots of atomic orbitals like 1s,2pz,3dz^2 by using angular part of hydrogen atom wave function.

(New experiments may be also be added)

References:

1. Findlay's Practical Chemistry – Revised by J.A. Kitchner (V^{th} edition)
2. Text Book of Quantitative inorganic analysis : A.I. Vogel.
3. Experimental Physical Chemistry : By F. Daniels and J. Williams
4. Experimental Physical Chemistry : R.C Das and B. Behera
5 Practical Physical Chemistry : B. Viswanathan and P.S. Raghavan

Learning Outcomes

1) Student should understand the practical's of physical chemistry.
2) Student must explore variety of instrumental experiments.
3) Student should understand physical properties through these experiments.

B. Analytical Chemistry

i) Physical Chemistry Section:

1 To determine formula of complex ion by Job's method by colorimetry.

2 Determine the solubility of lead iodide in presence of varying concentration of Salt KCl.

3 Determine the solubility of lead iodide in presence of varying concentration of Salt KNO_3

ii) Organic Chemistry Section

1 Analysis of pharmaceutical tablets: Ibrufen / INAH 2 Colorimetric estimation of drugs/dyes

3 Preparation of pesticides.

4 Column and thin layer chromatography

5 Interpretation of IR spectra.

iii) Inorganic Chemistry Section

1 To determine the amount of copper in brass metal alloy colorimetrically.

2 Separation and estimation of Copper and Cobalt on cellulose Column.

3 Separation and estimation of Nickel and Cobalt on a anion exchanger.

4 Separation and estimation of Iron and aluminium on a cation exchanger.

5 To determine the amount of iron in given soap sample by colorimetrically.

(New experiments may be also be added)

References:

1 A Text book of quantitative Inorganic Analysis – A. I. Vogel

2 Standards methods of Chemical Analysis-F.J. Welcher.

3 Experimental Inorganic Chemistry –W.G. Palmer.

4 Manual on Water and Waste Water Analysis, NEERI-Nagpur D.S. Ramteke and C.A. Moghe

5 Inorganic synthesis-King.

6 Synthetic Inorganic Chemistry-W.L. Jolly

7 EDTA Titrations–F. Laschka

Learning Outcomes

1) Student should understand the number of practicals like determine formula of complex ion by Job's method by colorimeter, Separation and estimation of Nickel and Cobalt on a anion exchanger, Preparation of pesticides.
2) Student must explore different concepts of practicals which is industrially important.
3) Student should understand applications of experimental chemistry.