।। सा विद्या या विमुक्तये ।।
स्वामी रामानंद तीर्थ मराठवाडा विद्यापीठ, नांदेड
"ज्ञानतीर्थ" परिसर, विष्णुपूरी, नांदेड - ४३१६०६ (महाराष्ट्र)
SWAMI RAMANAND TEERTH MARATHWADA UNIVERSITY NANDED
"Dnyanteerth", Vishnupuri, Nanded - 431606 Maharashtra State (INDIA)
Established on 17th September 1994 – Recognized by the UGC U/s 2(f) and 12(B), NAAC Re-accredited with 'A' Grade
25 1994 - 2019 SILVER JUBILEE YEAR

ACADEMIC (1-BOARD OF STUDIES) SECTION

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संलग्नित महाविद्यालयांतील विज्ञान व तंत्रज्ञान विद्याशाखेतील पदव्युत्तर स्तरावरील प्रथम वर्षाचे CBCS Pattern नुसारचे अभ्यासक्रम शैक्षणिक वर्ष २०१९–२० पासून लागू करण्याबाबत.

प रि प त्र क

या परिपत्रकान्वये सर्व संबंधितांना कळविण्यात येते की, **दिनांक ०८ जून २०१९ रोजी संपन्न झालेल्या ४४व्या मा. विद्या परिषद बैठकीतील ऐनवेळचा विषय क्र.११/४४–२०१९** च्या ठरावानुसार प्रस्तुत विद्यापीठाच्या **संलग्नित महाविद्यालयांतील विज्ञान व तंत्रज्ञान विद्याशाखेतील पदव्युत्तर स्तरावरील प्रथम वर्षाचे** खालील विषयांचे **C.B.C.S. (Choice Based Credit System) Pattern** नुसारचे अभ्यासक्रम शैक्षणिक वर्ष २०१९–२० पासून लागू करण्यात येत आहेत.

1. Bioinformatics
2. Biotechnology
3. Boichemistry
4. Botany
5. Chemistry
6. Computer Management
7. Computer Science
8. Dairy Science
9. Environmental Science
10. Herbal Medicine
11. Information Technology
12. M.C.A.
13. Microbiology
14. Physics
15. Software Engineering
16. System Administration & Networking
17. Zoology

सदरील परिपत्रक व अभ्यासक्रम प्रस्तुत विद्यापीठाच्या **www.srtmun.ac.in** या संकेतस्थळावर उपलब्ध आहेत. तरी सदरील बाब ही सर्व संबंधितांच्या निदर्शनास आणून द्यावी.

'ज्ञानतीर्थ' परिसर,
विष्णुपुरी, नांदेड – ४३१ ६०६.
जा.क्र.: शैक्षणिक–१/परिपत्रक/पदव्युत्तर–सीबीसीएस अभ्यासक्रम/२०१९–२०/**४६४**
दिनांक : ११.०७.२०१९.

स्वाक्षरित/–
उपकुलसचिव
शैक्षणिक (१–अभ्यासमंडळ) विभाग

प्रत माहिती व पुढील कार्यवाहीस्तव :

१) मा. कुलसचिव यांचे कार्यालय, प्रस्तुत विद्यापीठ.
२) मा. संचालक, परीक्षा व मूल्यमापन मंडळ यांचे कार्यालय, प्रस्तुत विद्यापीठ.
३) प्राचार्य, सर्व संबंधित संलग्नित महाविद्यालये, प्रस्तुत विद्यापीठ.
४) साहाय्यक कुलसचिव, पदव्युत्तर विभाग, प्रस्तुत विद्यापीठ.
५) उपकुलसचिव, पात्रता विभाग, प्रस्तुत विद्यापीठ.
६) सिस्टम एक्सपर्ट, शैक्षणिक विभाग, प्रस्तुत विद्यापीठ.

Swami Ramanand Teerth Marathwada University, Nanded-431606

स्वामी रामानंद तीर्थ
मराठवाडा विद्यापीठ,नांदेड.

Syllabus of M.Sc. I yr. Chemistry

(CBCS PATTERN WITH W.E.F. 2019-20)

SEMESTER PATTERN

Post Graduate (PG) Programme in Chemistry,

Affiliated Colleges

Program specific outcome

1. To impart the chemistry knowledge of global standard
2. Global level opportunity for research and Ph.D. program
3. Discipline specific competitive examinations conducted by different organizations
4. Enormous job opportunities in chemical, pharmaceutical, food and material industries including academic institutions
5. Specific placement in R and D in various industries

Swami Ramanand Teerth Marathwada University

M. Sc. Chemistry Core and Elective papers

M. Sc. F. Y. (First Semester)

Sr. No.	Paper No.	Title	Contact hours	Credits
Core papers				
1.	CH-411	Inorganic Chemistry	60	4
2.	CH-412	Organic Chemistry	60	4
3.	CH-413	Physical Chemistry	60	4
4.	CH-414	Analytical chemistry	60	4
Practical courses				
5.	LCH-411	Inorganic Chemistry (Laboratory course 1)	120	4
6.	LCH-412	Organic Chemistry (Laboratory Course 2)	120	4
7.	SCH-410	Seminar	15	1

Elective Paper

1.	ECH-411	Bioorganic Chemistry	60	4

M. Sc. F. Y. (Second Semester)

Sr. No.	Paper No.	Title	Contact hours	Credits
Core papers				
1.	CH-421	Inorganic Chemistry	60	4
2.	CH-422	Organic Chemistry	60	4
3.	CH-423	Physical Chemistry	60	4
4.	CH-424	Analytical chemistry	60	4
Practical courses				
6.	LCH-413	Physical Chemistry (Laboratory course 1)	120	4
7.	LCH-414	Analytical Chemistry (Laboratory Course 2)	120	4
8.	SCH-220	Seminar	15	1

Elective Paper

1.	ECH-421	Biophysical Chemistry	60	4

Swami Ramanand Teerth Marathwada University

M. Sc. Chemistry Core and Elective papers drafts

M. Sc. F. Y. (First Semester)

Semester	Paper No.	Course No.	External (ESE)	Internal (CA)	Total
Ist	I	CH-411	75 Marks (Credit–3)	25 Marks (Credit–1)	100 Marks Credit–4
	II	CH-412	75 Marks (Credit–3)	25 Marks (Credit–1)	100 Marks Credit–4
	III	CH-413	75 Marks (Credit–3)	25 Marks (Credit–1)	100 Marks Credit–4
	IV	CH-411	75 Marks (Credit–3)	25 Marks (Credit–1)	100 Marks Credit–4
	V	ECH-411	75 Marks (Credit–3)	25 Marks (Credit–1)	100 Marks Credit–4
	Seminar	SCH-410	-	25 Marks (Credit–1)	25 Marks (Credit–1)

For Internal (CA) : (2 tests 15 Marks) + (Assignments – 10 Marks)

M. Sc. F. Y. (Second Semester)

Semester	Paper No.	Course No.	External (ESE)	Internal (CA)	Total
IInd		CH-421	75 Marks (Credit–3)	25 Marks (Credit–1)	100 Marks Credit–4
		CH-422	75 Marks (Credit–3)	25 Marks (Credit–1)	100 Marks Credit–4
		CH-423	75 Marks (Credit–3)	25 Marks (Credit–1)	100 Marks Credit–4
		CH-424	75 Marks (Credit–3)	25 Marks (Credit–1)	100 Marks Credit–4
		ECH-421	75 Marks (Credit–3)	25 Marks (Credit–1)	100 Marks Credit–4
	Seminar	SCH-220	-	25 Marks (Credit–1)	25 Marks (Credit–1)

For Internal (CA) : (2 tests 15 Marks) + (Assignments – 10 Marks)

M. Sc. F. Y. (Lab Course)

Paper No.	Course No.	External (ESE)	Internal (CA)	Total
XI	LCH-411	75 Marks (Credit–3)	25 Marks (Credit–1)	100 Marks Credit–4
XII	LCH-412	75 Marks (Credit–3)	25 Marks (Credit–1)	100 Marks Credit–4
XIII	LCH-413	75 Marks (Credit–3)	25 Marks (Credit–1)	100 Marks Credit–4
XIV	LCH-414	75 Marks (Credit–3)	25 Marks (Credit–1)	100 Marks Credit–4

Total credit : Sem. – I + Sem. II + Lab. Course + Elective + Seminar =

16 + 16 + 16 + 08 + 02 = 58

SWAMI RAMANAND TEERTH MARATHWADA UNIVERSITY, NANDED
CHOICE BASED CREDIT SYSTEM (CBCS) SEMESTER PATTERN
Post Graduate (PG) Programme in Chemistry

SYLLABUS FOR M.Sc. PART – I
M. Sc. Chemistry
SEMESTER PATTERN
2019-2020

M. Sc. First Year, Semester-I
Inorganic Chemistry - I
Paper : I (CH-411)
Credit - 04

Marks : 75 60 P

OBJECTIVES:

1. To look at the evidence and experiments that are used in the analysis of the reaction pathways of metal complexes.
2. To understand the concepts of organometallic chemistry, coordination chemistry, and material chemistry to catalysis.
3. To understand the nature and bonding in metal complexes with spectroscopic methods
4. To understand how different elements are taken up selectively by different cells and intracellular compartments and structure and function of complexes and material that are formed in the biological environment. .
5. To motivate students for higher education.

1. **Reactions of metal complexes (Part first)** 20P

Introduction.

Lible and Inert complexes.
VBT explanation of libility and inertness.
Taube's explanation of libility and inertness.
Ligand substitution reactions.
SN1 : substitution, nucleophilic, unimolecular mechanism (Dissocitive mechanism) : Introduction, Characteristics, Example.
SN2 : substitution, Nulcleophilic, Bimolecular Mechanism (Associative mechanism): Introduction, Characteristics, Example.
SN1 CB : Substitution Nucleophilic Unimolecular Conjugate Base Mechanism : Characteristics, Example.
Anation Reaction.
Electron-transfer reactions (Redox reaction): Introduction with example.
Outer sphere mechanism, tunneling mechanism, essential requisite for electron transfer, factors which favour outer sphere electron transfer reactions.
Inner-sphere mechanism, characteristics, example, proof for innersphere mechanism, inner sphere mechanism and bridging ligand, inner sphere mechanism and electronic configuration.

2. Chemistry of nanomaterials and nano science 20 P

Introduction :

Terminology, optical properties of nonmaterials, characterization methods, top down and bottom-up fabrication, templeted synthesis using frameworks, supports and substrates, self assembled nanostructures , control of nanoarchitecture, one dimensional control, two dimensional control, three dimensional control, bioinorganic nanomaterials, DNA and nanomaterials, natural and artificial nanomaterials and bionanocomposites.

3. Electronic Absorption spectra of transition metal complexes 20P

Introduction, Basis of electron absorption

Spin orbit coupling : i) Russell-sounder coupling ii) j-j- coupling

Microstates and its calculations from

i) the number of orbital and number ofelectron ii) Orbital degeneracy, spin degeneracy and number of unpaired electrons

Term Symbols : Rules for determining term symbols ,Hund's rule for deciding the relative energies of term symbols (Hund's First,Second And third rule)

Determination of ground States, Hole formation, Symmetry species of terms

Selection rules : I) Laporte selection rule ii) Spin section rules

Spectra of transition metal complexes : splitting of terms, Orgel diagrams for tetrahedral and octahedral complexes, Orgel correlation diagrams, Tanabe –Sugano correlation diagrams (T-S diagrams) for d^2,d^3 configurations, Comparison between Orgel and T-S diagrams .

Nephelauxetic effect, Nephelauxetic ratio(β) and Nephelauxetic series.

Charge transfer spectra : LMCT, MLCT and charge transfer in complexes having metal in mixed valence state (Metal to metal charge transfer)

Comparison between d-d transition and charge transfer spectra.

Magnetic properties of complexes : i) cooperative magnetism ii) spin crossover complexes

Reference Books :

1. Advanced Inorganic Chemistry, F.A. Cotton and Wilkinson, John Wiley.
2. Inorganic Chemistry, J.E. Huhey, Harpes and Row.
3. Inorganic Electronic Spectroscopy, A.B.P. Lever, Elsevier.
4. Magneto chemistry, R.L. Carlin, Springer Verlag.
5. Comprehensive Coordination Chemistry eds, G. Wilkinson, R.D. Gillars and J.A. McCleverty, Pergamon.
6. Advanced Inorganic Chemistry : Satyaprakash, J.D. Tuli, Version I S.K. Basu and R.D. Madan.
7. Advanced Inorganic Chemistry : Vol. I and II Gurudeep Raj.
8. Concise Inorganic Chemistry : J.D. Lee.
9. Principles of Inorganic Chemistry : Puri, Sharma and Kalia.
10. Inorganic Chemistry (Principles, structures and reactivity) (4th Edition): J.E. Huheey, E.A. Keitler and R.L. Keitler.
11. Inorganic Chemistry 3rd Edition : G.Y. Miessler and D.A. Tarr.
12. Selected topics in Inorganic Chemistry : W.U. Malik, J.D. Tuli and R.D. Madan.
13. Chemistry of the elements : N.N. Greenwood and A. Earnshaw.
14. Symmetry and Spectroscopy of molecules : K. Veera Reddy.
15. Inorganic Chemistr : Attkin and Shriver.
16. Some Aspects of Crystal Filed Thoery : T.M. Dunn, D.S. Mcclure and R.G. Person.
17. Introduction to Ligand Fild: B.N. Figis

Outcome: Student will be able to

1. Learn various approaches in analyzing structures of simple molecules.
2. Understand the proposed pathways for reactions taking place in coordination complexes such as substitution reactions, redox reactions etc. and the various factors affecting to rates of these reactions.
3. Learn about mechanisms proposed for reactions taking place in coordination complexes, and will be able to understand to explain the product formation based on these mechanisms.
4. Understand how to construct molecular orbital diagrams for simple molecules as well as coordination complexes.
5. Draw molecular orbital diagrams for sigma and pi bond formation in coordination complexes and will be able to understand and explain the difference between respective molecular orbital diagrams.

M. Sc. First Year, Semester-I
Organic Chemistry - I
Paper : II (CH-412)
Credit - 04

Marks : 75 **60 P**

Objectives :

- Students should learn about Nature of Chemical bonding in Organic molecules, Structure and Reactivity.
- To understand the various concept of Stereochemistry, Asymmetric synthesis, absolute configuration and Conformation analysis.
- To explain the mechanism of aliphatic electrophilic and nucleophilic substitution reactions.
- To interpret the problems of Benzenoid and Non Benzenoid compounds.
- Students develop the knowledge of Thermodynamic of the reaction and Kinetic of the reactions
- Student should explain the Free radical mechanism.
- To develops skill of writing mechanism.

1. Nature of Bonding in Organic Molecules: **10 P**

Delocalised chemical bonding –conjugation, cross-conjugation, resonance, hyperconjugation, tautomerism. Aromaticity in benzenoid and non-benzenoid compounds, alternant and non-alternant hydrocarbons, Huckel's rule, energy level of π-molecular orbitals, annulenes, anti-aromaticity, homo-aromaticity. Study of Structure of compounds crown ether complexes, cryptands, inclusion compounds, cyclodextrins, catenanes and rotaxanes.

2. Stereochemistry: **12 P**

Stereo chmical principles : Enantiometric relationships, Distereomeric relationships, R and S, E and Z nomenclature, Dynamic stereochemistry, Prochiral relationships. Homotopic, enantiotopic, groups and faces, Stereo-specific and stereo-selective reactions.

Conformational analysis of halo, hydroxy and methyl mono and disubstituted Cyclohexane, decalins, effect of conformation on reactivity, conformation of glucose and fructose. Elements of symmetry, chirality, molecules with more than one chiral center, threo and erythro isomers, optical purity, enantiotopic, and diasteretopic atoms, groups and faces, stereospecific and stereoselective synthesis. Asymmetric synthesis. Optical activity in absence of chiral carbon (biphenyls, allenes and spiranes), chirality due to helical shape, Methods of resolution and recemic modification.

3. Reaction Mechanism: Structure and activity: **10 P**

Types of mechanism, types of reaction, thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammond's postulate. Potential energy diagrams, transition state and intermediates, methods of determining mechanism, isotope effects. Generation, structure and stability of carbocations, carbanions, free radicals, carbenes and nitrenes. Effect of structure on reactivity – Resonance and field effect, steric effect, quantitative treatment. The Hammett equation and linear free energy relationship, substituents and reaction constants. Taft equation.

4. Aliphatic Nucleophilic Substitution: 12 P

The SN^2, SN^1, mixed SN^1 and SN^2 and SET mechanism. The neighbouring group mechanism, neighbouring group participation by π and σ bonds, anchimeric assistance. The SN^i mechanism. Nucleophilic substitution at an allylic, aliphatic and a vinylic carbon. Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium. Phase transfer catalysis, ambident nucleophile, regioselectivity, Classical and nonclassical carbocations, phenonium ions, norbornyl system.

5. Aromatic nucleophilic Substitution: 8 P

SN^{Ar}, SN^1, benzyne and SRN^1 mechanism. Reactivity – effect of substrate structure leaving group and attacking nucleophile. Sommelet-Hauser and Smiles rearrangements.

Home assignment: Von Richter rearrangement reaction.

6. **Elimination Reaction : 8 P**

The E^2, E^1 and E^1CB mechanisms and their spectrum. Orientation of the double bond. Reactivity – effects of substrate structures, attacking base, the leaving group and the medium. Mechanism and orientation in pyrolytic elimination.

7. Home assignment: Allylic halogenation (NBS), oxidation of aldehydes to carboxylic acids, auto-oxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salts. Sandmeyer reaction. Free radical rearrangement. Hunsdiecker reaction.

Books:

1. Advanced Organic Chemistry-Reaction Mechanism and structure, Jerry March, John Wiley.
2. Advanced Organic Chemistry, F.A. Carey and R.J. Sundberg, Plenum.
3. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman.
4. Structure and Mechanism in Organic Chemistry, C.K. Ingold, Cornell University press.
5. Organic Chemistry, R.T. Morrison Boyd, Prentice-Hall.
6. Modern Organic Reactions, H.O. House, Benjamin.
7. Principles of Organic Synthesis, R.O.C. Norman and J.M. Coxon, Blackie Academic and Professional.
8. Reaction Mechanism in Organic Chemistry, S. M. Mukherji and S.P. Singh, Macmillan.
9. Stereochemistry of Organic Compounds, D. Nasipuri, New Age International.
10. Stereochemistry of Organic Compounds, P. S. Kalsi, New Age International.

Outcome: Student will be able to

- Understand the various types of Reaction Mechanism.
- Adopt the concept of Bonding in Organic Molecules.
- Learn the concept of Stereochemistry and to identify the Stereo chemical reactions.
- Explain the various problems of aromaticity, homoaromaticty and antiaromaticity.
- Familiarize the various types of Substitution reactions and their mechanism
- Gain knowledge of free radical reactions.
- Justifies the various effect of substrate.

M. Sc. First Year, Semester-I
Physical Chemistry - I
Paper : III (CH-413)
Credit - 04

Marks : 75 **60 P**

Objective:

- To understand the basic concepts, laws and postulates of quantum mechanics
- To understand the concept of wave functions and operators and to solve Schrodinger wave equation for rigid rotor, harmonic oscillator and for hydrogen atom
- To understand the concept of angular momentum and electronic structure of atoms
- To understand laws of thermodynamics, concept of partial molar properties and non-ideal systems
- To understand the distribution and thermodynamic probability and to discuss the partition functions and its significance
- To relate entropy production in different system and understand Onsager's relations
- Develop skill in problems solving

1. Quantum Chemistry: **20P**

A) Introduction to Exact Quantum Mechanical Results:

a) The postulates of quantum mechanics.

b) Schrödinger equation in Laplacian and Hamiltonian form. Significance of Eigen –values and Eigen functions. Significance of Ψ and Ψ^2.

c) Discussion of solutions of the Schrödinger equation to

i. Particle in one dimensional box,

ii. Particle in three dimensional box,

iii. Harmonic oscillator,

iv. The rigid rotator and

v. Hydrogen and Hydrogen like systems.

d) Orthogonality and normalisation of wave functions.

e) Numericals on (c) and (d).

B) Approximate Methods:

a) The variation theorem, linear variation principle.

b) Perturbation theory (first order and non degenerate).

C. Angular Momentum:

a) Ordinary angular momentum, generalized angular momentum, eigen functions for angular, Momentum, eigen values of angular momentum.

b) Spin, anti-symmetry and Pauli's exclusion principle, commutation elation, Zeeman splitting, Spin orbital coupling and R-S couplings.

c) Operator using ladder operators, addition of angular momentum.

Home assignment for students: Application of Schrödinger equation to hydrogen atom. Applications of variation method and perturbation theory to the Helium atom.

2. Phase Rule : 07P

a) Recapitulation of phase rule and terms involved in it.

b) Three component system: representation of ternary systems.

c) Partially miscible three liquid systems:- 1) system composed of three liquid components, one partially miscible pairs, two partially miscible, three partially miscible pairs. 2) System composed of two solid and a liquid components:- formation of eutectic systems, crystallization of pure components only, formation of binary compounds, one double salt formation .

Home assignment for students: formation of binary compounds hydrate formation, formation of ternary compounds, formation of solid solutions, partially miscibility of phases.

3. Thermodynamics : 20P

A. Classical Thermodynamics:

a) Brief resume of concepts of laws of thermodynamics. Free energy and entropies.

b) Partial molar, partial molar free energy chemical potential, partial molar volume and partial molar heat content and their significances. Determinations of these quantities.

c) Concept of fugacity and determination of fugacity by graphical method and from equation of state.

d) Non-ideal systems : Excess functions for non-ideal solutions.

e) Activity, activity coefficient. Debye-Huckel theory for activity coefficient of electrolytic solutions, determination of activity and activity coefficients by 1) solubility 2) E.M.F. method. 3) vapour pressure method, Ionic strength.

B. Statistical Thermodynamics :

a) Concept of distribution, thermodynamics probability, ensemble averaging, postulates of ensemble averaging. Canonical, grand canonical and micro-canonical ensembles.

b) Partition functions: Translational, rotational, vibrational and electronic partition functions. calculation of thermodynamic properties in terms of partitionfunctions.

c) Applications of partition functions.

d) Numericals on A(e), B(b)

Home assignment for students : a) Corresponding distribution laws (Max well-Boltzaman distribution law **b)** Heat capacity behaviour of solids –chemical equilibria constant in terms of partition functions.

4. Crystallography 05 P

a) Solid state defects.

b) Semiconductors, N and P type, effect of temperature on N and P type Semi conduction.

c) Packing of uniform spears, octahedral and tetrahedral voids(holes), close packing of spear.

d) Isomorphism, lattice energy and born haber cycle.

5. Electrochemistry I **08 P**

a) Anomaly of strong electrolytes, Deby-Huckel theory, Onsager equation, & its verification wine effect, Deby falkenhagen effect, ion solvent, intractions.

b) Thermodynamics of electrified interface equation, Derivation of electro capillary, Lippmann equation (surface excess)

c) Structure of electrified interfaces equation, Electrical double layer, Theories of structure of Electrical double layer. Helmoholtz-perrin. Gouy-Chapman theory, Stern's theory.

Books Suggested

1. Physical Chemistry -P.W. Atkins, ELBS.
2. Introduction to Quantum Chemistry -A.K.Chandra,Tata McGraw Hill.
3. Quantum Chemistry - Ira N.Levine, Prentice Hall.
4. Coulson's Valence -R. McWeeny ELBS.
5. Chemical Kinetics -K.J.Laidler, McGraw Hill.
6. Kinetics and Mechanism of Chemical Transformations -J.Rajaraman and J.Kuriacose, Macmillan.
7. Micelles, Theoretical and Applied Aspects - V.Moroi, Plenum
8. Modern Electrochemistry Vol.I & II, J.O.M. Bockris & A.K.N. Reddy, Plenum
9. Introduction to Polymer Science - V.R.Gowarikar, N,V.Vishwanathan & J.Sridhar, Wiley Eastern.

Outcome: The students will be able to

- Explain basic concepts, laws and postulates of quantum mechanics
- Describe different wave functions and operators
- The Schrodinger wave equation for the calculation of Energies of rigid rotor and harmonic oscillator and solve it for hydrogen atom
- Explain the concept of angular momentum
- Describe the electronic structure of atoms
- Good overview of laws of thermodynamics, partial molar properties for different systems and concept and examples of non-ideal systems
- Discuss concept distribution with examples, they will be able to explain most probable distribution and thermodynamic probability
- Concept of partition functions and its significance
- Can relate and explain the entropy production in different system and understand Onsager's relations
- Solve problems related to quantum chemistry, will have large horizon of critical thinking and analytical reasoning

M. Sc. First Year, Semester-I
Physical Method in Chemistry
Paper : IV (CH-414)
Credit - 04

Marks : 75 **60 P**

Objectives:

- To introduce the concepts of symmetry.
- Study the concept of group theory for understanding molecular representations,
- To provide an introductory treatment of bonding theories, electronic and vibrational spectroscopy.
- Molecular Symmetry, Symmetry operations and symmetry elements: Plane of symmetry, Proper/Improper Axis of symmetry, Inversion center, Identity element.

Course contents

1. Symmetry and Group Theory in Chemistry **15P**

Symmetry elements and symmetry operation, definitions of group, subgroup, relation between orders of a finite group and its subgroup. Conjugacy relation and classes. Point symmetry group. Schonfiles symbols, representations of groups by matrices (representation of the C_n, C_{nv}, C_{nh}, D_{nh} etc. groups to be worked out clearly.) Character of a representation. The great orthogonality theorem (without proof) and its importance. Character tables C_{1h}, C_{2V}, C_{3V} and their use.

2. Computer for Chemist **20P**

A. Introduction to computers and computing:

Basic structure and functioning of computers with a PC as an illustrative example. Memory, I/O devices. Secondary storage. Computer languages. Operating system with DOS as an example. Introduction to UNIX and WINDOWS. Data processing, principles of programming. Algorithms and flow-charts for chemical concepts.

B. Programming in Chemistry:

Development of small computer codes involving simple formulae in chemistry, such as Vander Waal's equation, pH titration, kinetics, radioactive decay.

3. **X-ray Diffraction** **15P**

Bragg condition. Miller indices, Laue method, Bragg method, Debye-Scherrer method of X-ray structural analysis of crystals, index reflections, identification of unit cells from systematic absences in diffraction pattern. Structure of simple lattices and X-ray intensities, structure factor and its relation to intensity and electron density, phase problem. Description of the procedure for an X-ray structure analysis, absolute configuration of molecules, Ramachandran diagram. Numerical on Braggs equation.

$n\lambda=2dSin\theta$

4. Electron Diffraction: **5P**

Scattering intensity vs. Scattering angle, Wierl equation, measurement technique, elucidation of structure of simple gas phase molecules with suitable examples.

Home assignment for students: Low energy electron diffraction and structure of surfaces.

5. Neutron Diffraction **5P**

Scattering of neutrons by solids and liquids, magnetic scattering, measurement techniques.

Home assignment for students: Elucidation of structure of magnetically ordered unit cell, applications.

Books Suggested

1. Physical Methods in Chemistry - R.S. Drago, Saunders College.
2. Chemical Applications of Group Theory - F.A. Cotton.
3. Basic Principles of Spectroscopy - R. Chang, McGraw Hill.
4. Computers and common Sense, R. Hunt and J. Shelly, Prentice Hall.
5. Computational Chemistry, A. C. Norris.
6. An introduction to digital computer design, V. Rajaram and T. Radhakrishnan, Prentice Hall.
7. Microcomputer Quantum Mechanics, J.P. Killngbeck, Adam Hilger.

Outcome: Students will be able to

- Understand how to recognize symmetry elements in a molecule.
- Assign the point group to a molecule.
- Deal with degenerate and non-degenerate representations.

Bioorganic Chemistry (Elective)
Paper : V (ECH-411)
Credit - 04

Marks : 75 **60 P**

Objectives:

- **know about the macromolecules in the biological systems and mode of functioning.**

1 Cell Structure and Functions: **1OP**

Structure of prokarytic and eukaryotic cells, intracellular Organelles and their functions, comparison of plant and animal cells Overview of metabolic processes-catabolism and anabolism. ATP-the biological energy currency. Origin of life-unique properties of carbon, chemical evolution and rise of living systems. Introduction to biomolecules, building blocks of bio-macromolecules.

2 Carbohydrates: **10P**

Conformation of monosaccharides, strucute and functions of PImportant derivatives of minosaccharides like glycosides, deoxy sugars, myoinosito, amino sugars. N-acetylmuramic acid, sialic acid, disaccharides and polysaccharides. Structural polysaccharides – cellulose and chitin. Storage polysaccharides-starch and glycogen. Structure and biological functions of glucosaminoglycans or mucopolysaccharides. Carbohydrates of glycoproteins and glycolipids. Role of sugars in biological recognition. Blood group substances. Ascorbic acid. Carbohydrate metabolism – Kreb's cycle, applications of carbohydrates.

3 Lipids: **1OP**

Fatty acids, essential fatty acids, structure and function of triacylglycerols. Glycerophospholipids ,sphiningolipids, cholesterol, bile acides prostaglandins. Lipoproteins composition and function, role in atherosclerosis. Propertieof lipid aggregates-micelles, bilayers, liposomes and their possible biological functions. Biological membrages. Flid mosaic model of membrane structure. Lipid metabolism–B-oxidation of fatty acids.

4 Amino-acids, Peptides and Proteins : **10 P**

Chemical and enzymatic hydrolysis of proteins to peptides, amino acid sequencing. Secondary strucutre of proteins, forces responsible for holding of secondary structures. A-helix, b-sheets, super secondary structure, triple helix structure of collagen, Tertiary structure of protein-folding and domain structure. Quaternary structure. Amino acid metabolism-degradation and biosynthesis of amino acids, sequencedetermination: Chemical/enzymatic/mass spectral, racemization/ detection. Chemistry of oxyocin and tryptophan releasing hormone 9TRH).,

5 Nucleic Acids: **10P**

Purine and pyrimidine bases of nucleic acids, base pairing via H-bonding. Structure of ribonucleic acids (RNA) and deoxyribonucleic acids (DNA), double helix model of DNA and forces responsible for holding it. Chemical and enzymatic hydrolysis of nucleic acids. The chemical basis for heredity, and overview of replication of DNA, transcription, functions of nucleotides. Chemical synthesis DNA

6 **Enzymes and Enzyme Models:** **10P**

(a) Enzymes: Introduction and historical perspective, chemical and bioogical catalysis, remarkable properties of enzymes like caalytic power, specificity and regulation. Nomenclature and classification, extraction and purification. Fischer's

lock and key and koshland's induced fit hypothesis, concept and identification of active site by the use of inhibitors, affinity labeling and enzyme modification by site-directed mutagenesis. Enzyme kinetics, Michaelis–Menten and Lineweaver Burk plots, reversible and irreversible inhibition, mechanism of enzyme action. : Transition state theory, orientation and sterioc effect, acid base catalysis, coalent catalysis, strain or distortion some typical examples, enzyme in organic synthesis. (b) Enzyme Models: Host-guest chemistry, chiral recognition and catalysis, molecular recognition, molecular asymmetry and prochirality. Biomimetic chemistry, crown ethers, Cyclodextirns, cyclodextrin-based enzyme models, micelles, synthetic enzymes or synzymes.

Books

1. Principles of Biochemistry, A. A. Lehninger, Worth publishers.
2. Biochemistry, L. Stryer, W. H. Freeman.
3. Biochemistry, J. David Rawn. Neil Patterson.
4. Principles of Biochemistry, A. A. Lehninger, Worth publishers.
5. Biochemistry, L. Stryer, W. H. Freeman.
6. Biochemistry, J. David Rawn. Neil Patterson.
7. Biochemistry, oet and Voet, John Wiley.
8. Outlines of Biochemistry, E.E. Conn and P. K. Stumpf, John Wiley.
9 Bioorganic Chemistry A Chemical Approach to Enzyme Action, Hermann Dugas & C. Penny, Springer –Verla Understanding Enzymes, Trevor palmer, Prentice Hall.
9. Enzyme Chemistry Impact and Applications, Ed. Collin J. Suckling, Chapman and Hall
10. Enzyme Mechanisms Ed. M. I. Page and A. Williams, Royal Society of Chemistry.
11. Fundamentals of Enzymology, N. C. Price ad L. Stevens, Oxford University Press.
12. Immobilized Enzymes: An Introduction and Applications in Biotechnology, Michael D. Trevan, John Wiley.
13. Enzymatic Reaction Mechanisms, C. Walsh, W. H. Freemain.
14. Enzyme Structure and Mechanism, A. Fresht, W. H. Freeman..
15. Biochemistry: The Chemical Reactions of Living Cells, D.E. Metzler, Academic Press.

Outcome:

The basic principles govering the metabolic reactions, energy pathwasys, functioning of catalytic systems , evolution of life and fundamental process governing it

M. Sc. First Year, Semester-II
Inorganic Chemistry
Paper : VI (CH-421)
Credit - 04

Marks : 75 **60 P**

Objectives :

1. To inspire students for research activities in all fields.
2. To inspire students to take enthusiastically part in class.
3. To make enable students for publications in reputed journals.
4. To work out interaction amongst students and skilled personalities from industries.
5. To make enable students for SET/NET/GATE examination.
6. To generate scientific attitude amongst students through various means.

1. **Reaction of Metal Complexes (Part second)** 10 P

Substitution reactions of square-planar complexes.
Evidence for associative type SN2 mechanism.
Trans effect, applications of trans effect. Theories of trans effect, the polarization theory, evidences in favour of the polarization theory, defect of this theory, the Pi-bonding theory.
Cis effect.

2. **Catalyst.** 15 P

Introduction, General principle and mechanism of catalytic reaction. Types of catalysts.
Homogeneous Catalysis : Hydrogenation of alkenes, Hydroformulation,
Methanol Carbonylation, Wacker oxidation of alkenes, Palladium-catalysed C-C bond forming reaction,
Heterogeneous catalysis : The nature of Heterogeneous catalysts, amonia synthesis, Sulfur dioxide oxidation, Fischer-Tropsch Synthesis, Alkene Polymerization, New directions in heterogeneous catalysis such as Tethered catalysts.

3. **Bioinorganic Chemistry:** 15 P

Biological importance of essential and non essential elements.
Na/K Pump.
Metalloporphyrins : Structure of porphyrin molecule.
Hameoglobin **:**Structure, function of haemoglobin. Myoglobin **:** Structure & function.
Difference between haemoglobin & Myoglobin.
Chlorophyll : Structure & function, Photosynethesis PS-I & PS-II.
Electron carrier proteins in biological system:

i. Iron sulfur proteins - Rubredoxin, ferrodoxin.
ii. Cytochrome : Structure & function.
iii. Iron storage protein : Ferritin.
iv. Iron transporting biomolecule : Transferrin, siderophores (Non Protein), hemerythrin and hemocyanins.

Biological enzymes : Nitrogenase and Superoxide dismuthases.
Vitamin B12 (Cynocobalanine), structure and function.

4. **Structural methods in inorganic chemistry** 20 P

a. **Vibrational spectroscopy**:

Introduction

Physical basis requirement for vibrational spectroscopy.

Number of modes of vibration.

Force constant concept in vibrational spectroscopy.

Application of vibrational spectroscopy with respect to change in spectra of donor molecule upon complexation.

b. **Electron spin resonance spectroscopy**:

Introduction, Basic principle

Hyperfine structure of ESR in isotropic system (Exampes).

EPR spectra of transition metal complexes as single crystals. Nuclear spin of metal ion.

Reference compound in ESR.

Frequency in ESR and g-splitting factor.(Numericals)

c. **Mossbauer spectroscopy**:

Introduction, Basic principle, Condition for the Mossbauer spectroscopy

Parameter from Mossbauer spectra, isomer shift and electrical quadruple interactions.

Structural deduction.(Illustration)

Mossbauer spectra of inorganic compound/ complexes

Reference Books :

1. Advanced Inorganic Chemistry, F.A. Cotton and Wilkinson, John Wiley.
2. Inorganic Chemistry, J.E. Huhey, Harpes and Row.
3. Inorganic Electronic Spectroscopy, A.B.P. Lever, Elsevier.
4. Magneto chemistry, R.L. Carlin, Springer Verlag.
5. Comprehensive Coordination Chemistry eds, G. Wilkinson, R.D. Gillars and J.A. McCleverty, Pergamon.
6. Advanced Inorganic Chemistry : Satyaprakash, J.D. Tuli, Version I S.K. Basu and R.D. Madan.
7. Advanced Inorganic Chemistry : Vol. I and II Gurudeep Raj.
8. Concise Inorganic Chemistry : J.D. Lee.
9. Principles of Inorganic Chemistry : Puri, Sharma and Kalia.
10. Inorganic Chemistry (Principles, structures and reactivity) (4th Edition): J.E. Huheey, E.A. Keitler and R.L. Keitler.
11. Inorganic Chemistry 3rd Edition : G.Y. Miessler and D.A. Tarr.
12. Selected topics in Inorganic Chemistry : W.U. Malik, J.D. Tuli and R.D. Madan.
13. Chemistry of the elements : N.N. Greenwood and A. Earnshaw.
14. Symmetry and Spectroscopy of molecules : K. Veera Reddy.
15. Physical Chemistry through Problems : Dogra and Dogra.
16. Inorganic Chemisstr : Attkin and Shriver.
17. Elements of Magnetochemistry : A. Samal and R.L. Datta.
18. Some Aspects of Crystal Filed Thoery : T.M. Dunn, D.S. Mcclure and R.G. Person.
19. Introduction to Magnetochemistry : Alan Earnshaw.
20. Introduction to Ligand Files : B.N. Figgis.
21. Physical methods in chemistry by Drago R.S.
22. Coordination chemistry by R.Gopan and V Ramlingam
23. Structural methods in inorganic chemistry by E A V Ebsworth, D W H Rankin and S Cradock

24. Infrared UV- Visible spectroscopy by Nakamoto.

Outcome: Students will be to

- Learn basic terms regarding electronic spectra of coordination complexes, interpretation of electronic spectra and various important parameters necessary for it, drawing of Orgel andT-S diagrams used for electronic spectra, prediction of possible electronic transitions present in electronic spectra of coordination complexes etc.
- He/she will understand magnetic nature of complexes, measurement of magnetic moment in coordination complexes, prediction of magnetic nature of complexes using spin only formula.
- He/she will learn the terms such as diamagnetic and paramagnetic nature of coordination complexes, difference between them, anomalous magnetic moments, spin cross over etc.
- He/she will understand the chemistry of carbonyl and nitrosyl molecules, their application as ligand molecules in complex formation, structure and bonding present in various carbonyl and nitrosyls complexes, applications etc.
- He/she will learn chemistry of boranes, carboranes and metal clusters, the concept of 3C-2e bond used to explain structural aspects in boranes and carboranes, polyhedral skeletal electron pair theory and its applications in explaining structures of metal clustes etc.

M. Sc. First Year, Semester-II
Organic Chemistry
Paper : VII (CH-422)
Credit - 04

Marks : 75 **60 P**

Objective

- Students should learn the mechanism of electophilic and Nucleophilic substitution reactions
- To develops the ability to apply the knowledge of addition and elimination reactions
- To adopt the knowledge of pyricyclic reactions and sigma tropic reaction. To expose the students to various chemical reactions
- To learn about the addition of C-C Multiple Bonds and Carbon-Hetero Multiple Bonds
- To adopt the skill of writing mechanism of some important name reactions

1. Aliphatic Electrophilic Substitution: 8P

Bimolecular mechanism - SE^2 & SE^i. The SE^1 mechanism, electrophilic substitution accompanied by double bond shift. Effect of substrates, leaving group and the solvent polarity on the reactivity.

2. Aromatic Electrophilic Substitution: 10P

The arenium ion mechanism, orientation and reactivity, energy profile diagrams. The ortho/para ratio, ipso attack. Quantitative treatment of reactivity in substrates and electrophiles. Diazonium coupling, Vilsmeir reaction, Gatter-Koch reaction.

3. Addition to Carbon – Carbon Multiple Bonds: 8P

Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, regioselectivity and chemoselectivity, orientation and reactivity. Addition to cyclopropane ring. Hydroboration, Michael reaction. Sharpless asymmetric Epoxidation.

Home assignment: Hydrogenation of double and triple bond, Hydrogenation of aromatic rings.

4. Addition to Carbon – Hetero Multiple Bonds: 1OP

Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acids, esters and nitriles. Addition of Grignard reagents, Organo-zinc and organo-lithium reagents to carbonyl and unsaturated carbonyl compounds. Wittig reaction. Mechanism of condensation reaction involving enolates- Aldol, Knoevenagel, Claisen, Mannich, Benzoin, Perkins and Stobbe reaction.

Home assignment: Hydrolysis of esters and amides, ammonolysis of esters.

5. Pericyclic Reactions: 12P

Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3- butadiene, 1,3,5-haxatriene and allyl system. Classification of pericyclic reactions. Woodward-Hoffmann correlation diagrams. FMO and PMO approach. Electrocyclic reactions-conrotatory and disrotatory motions, 4n, 4n +2 and allyl systems. Cycloadditions – antarafacial and suprafacial additions, 4n and 4n +2 systems, 2+2 addition of ketenes, 1,3 dipolar cycloadditions and cheleotropic reactions. Sigmatropic rearrangements - Suprafacial and antarafacial shifts of H, sigmatropic shifts involving carbon moieties,

3,3 and 5,5- Sigmatropic rearrangements. Claisen, Cope and aza-Cope rearrangements.

6. Photochemistry: 10P

Principles–photochemical theory, electronic excitation, singlet and triplet states, Jablonski diagram. Energy transfer, quantum efficiency.

a) Photochemistry of carbonyl compound: Photoreduction, Norrish type–I & II, Paterno-Buchireaction.
b) Photochemistry of α, β-unsaturated ketones.
c) Photochemistry of olefins: cis-trans isomerism.
d) Miscellaneous photochemical reaction: Photo-fries reaction of anilides, Photo rearrangements, Barton reaction singlet molecular oxygen reaction Photochemical formulation of smog photo-degradation of polymers, photochemistry of vision, nπ- pπ rearrangement.

7. Home assignment: Functional group transformations, functional tautomerism and ene reactions.

Books:

1. Advanced Organic Chemistry-Reaction Mechanism and structure, Jerry March, John Wiley.
2. Advanced Organic Chemistry, F.A. Carey and R.J. Sundberg, Plenum.
3. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman.
4. Structure and Mechanism in Organic Chemistry, C.K. Ingold, Cornell University Press.
5. Organic Chemistry, R.T. Morrison Boyd, Prentice-Hall.
6. Modern Organic Reactions, H.O. House, Benjamin.
7. Principles of Organic Synthesis, R.O.C. Norman and J.M. Coxon, Blackie Academic and Professional.
8. Pericyclic Reactions, S. M. Mukherji, Macmillan, India.
9. Reaction Mechanism in Organic Chemistry, S. M. Mukherji and S.P. Singh, Macmillan.
10. Stereochemistry of Organic Compounds, D. Nasipuri, New Age International.
11. Stereochemistry of Organic Compounds, P. S. Kalsi, New Age International.

Outcome: Students will be able to

- Gain the knowledge of addition reaction between a hetero atom and double bonded carbon compounds.
- Learn familiar name Reaction
- Obtain an outline about mechanism of Aromatic Substitution reactions
- Know synthetically the process relevant Organic –Chemical reactions and be able to discuss the mechanism of these reactions.
- Understand the skill of solving problems of pericyclic reactions
- Get the clear picture of about pyricyclic reactions

M. Sc. First Year, Semester-I
Physical Chemistry
Paper : VIII (CH-423)
Credit - 04

Marks : 75 **60 P**

Objective:

- To understand concepts and properties of surfactants and macromolecules
- To state laws, principles, theories related to the electrochemistry of the solutions
- To discuss and understand the corrosion, its monitoring and presentation
- To discuss different theories of reaction rates
- To understand the kinetics of complex reactions, catalysis etc.
- To perform the calculations and solve the numerical of electrochemistry and chemical kinetics
- To develop skill in problems solving, critical thinking and analytical reasoning

1. Surface Chemistry: **24P**

A. Adsorption:

a) Surface tension, capillary action, pressure difference across curved surface (Laplace equation).

b) Gibbs adsorption isotherm.

c) BET equation and estimation of surface area.

d) Surface films on liquids (Electro-kinetic phenomenon) and catalytic activity at surfaces.

Home assignment for students : Kelvin equation for vapour pressure of droplets.

B. Micelles :

a) Surface active agents, classification of surface active agents.

b) Micellisation, hydrophobic interaction, critical miceller concentration (CMC), factors affecting the CMC of surfactants, counter ion binding to micelles, thermodynamics of micellisation - phase separation and mass action models.

Home assignment for students : solubilisation, micro emulsion reverse micelles.

C. Macromolecules:

a) Polymers - definition, types of polymers, electrically conducting, fire resistant, liquid crystal polymers.

b) kinetics of polymerization, mechanism of polymerization.

c) Difference between polymers and macromolecules.

d) Molecular mass, number and mass average molecular mass, molecular mass determinations by i) osmometry, ii) viscometry, iii) diffusion and iv) light scattering methods.

Home assignment for students: Sedimentation, chain configuration of macromolecules, calculation of average dimensions of various chain structures.

2. Electrochemistry-II: 16P

a) Over potential, types of over potentials.

b) Exchange current density, Derivation of Butler-Volmer equation, Tafel plot.

c) Semi conductor interface. Theory of double layer at Semi conductor, electrolyte solution Interface, effect of light at semiconductor, Solution interface.

d) Polarography, Theory, instrumentation, working and applications of the technique.

e) Introduction to corrosion, homogenous theory, forms of corrosion, Corrosion monitoring and prevention methods

Home assignment for students:

a) Quantum aspect of charge transfer at electrodes –solution interfaces, quantization of charge transfer, tonnelling

b) Electro catalysis influence of various parameters. Hydrogen electrodes,

c) Biochemistry, Threshold membrane phenomenon, Nernst-Plank equation.

3. Chemical Dynamics: 20P

a) Methods of determining rate laws – i) Differential method and ii) Fractional change method.

b) Theories of reaction rates – i) collision theory of reaction rates, steric factor, ii) Transition state theory, thermodynamic formulation of TST.

c) Ionic reactions, kinetic salt effects.

d) Dynamic chain (Kinetics of the reactions, thermal/photochemical) – i) pyrolysis of acetaldehyde , ii) decomposition of ethane, iii) hydrogen-chlorine reaction, iv) hydrogen-bromine reaction.

e) Oscillatory reactions (Belousov-Zhabotinsky reaction).

f) Enzyme catalysis, kinetics of enzyme reactions, Michalis - Menten equation.

g) General features of fast reactions, study of fast reaction by flow method. Flash photolysis and the nuclear magnetic resonance method.

h) Dynamics of unimolecular reactions - i) Lindemann hypothesis ii) Hinshelwood theory iii) K-R-R treatment and iv) slater's theory . i) Numricals on (a) and (b).

Home assignment for students : a) Steady state kinetics, kinetic and thermodynamic control of reactions, treatment of unimolecular reactions. b) Dynamics and molecular motions, probing the transition state, dynamics of barrierless chemical reactions in solution. c) Dynamics of unimolecular reactions (Rice-Ramsperger-Kassel - Marcus [RRKM] theory of unimolecular reactions.)

Books Suggested

1. Physical Chemistry -P.W. Atkins, ELBS.
2. Introduction to Quantum Chemistry -A.K.Chandra,Tata McGraw Hill.
3. Quantum Chemistry - Ira N.Levine, Prentice Hall.
4. Coulson's Valence -R. McWeeny ELBS.
5. Chemical Kinetics -K.J.Laidler, McGraw Hill.
6. Kinetics and Mechanism of Chemical Transformations -J.Rajaraman and J.Kuriacose, Macmillan.

7. Micelles, Theoretical and Applied Aspects - V.Moroi, Plenum
8. Modern Electrochemistry Vol.I & II, J.O.M. Bockris & A.K.N. Reddy, Plenum
9. Introduction to Polymer Science-V.R.Gowarikar, N,V.Vishwanathan & J.Sridhar, Wiley Eastern.
10. Advanced physical chemistry – J.N. Gurtu & A. Gurtu, A Pragati Edition.

Outcome: Students will be able to

- Understand the basic concepts and properties of surfactants and macromolecules
- State and apply different laws, principles, theories related to the electrochemistry of the solutions.
- Discuss and apply the information about corrosion, its monitoring and presentation.
- Distinguish different theories of reaction rates.
- Understand the kinetics of complex reactions, catalysis etc.
- Perform the calculations and solve the numerical of electrochemistry and chemical kinetics.
- Develop skill in problems solving, critical thinking and analytical reasoning.

M. Sc. First Year, Semester-I
Principles of Spectroscopy
Paper : IX (CH-424)
Credit - 04

Marks : 75 **60 P**

Objective:

- This course aims to introduce the basic principles of spectroscopy
- To understand how of electromagnetic radiations in certain region energy interact with the matter.
- To understand principles behind these techniques and interaction of radiation with the matter.
- To interpret the rotational, vibration and electronic spectra of simple molecules.

Course contents

1. Unifying Principles: 7P

Electromagnetic radiation, interaction of electromagnetic radiation with matter-absorption, emission, transmission, reflection, refraction dispersion, polarisation and scattering. Uncertainty relation and natural line width and natural line broadening, transition probability, results of the time dependent perturbation theory, transition moment, selection rules, intensity of spectral lines.

Home assignment for students: Born-Oppenheimer approximation rotational, vibrational and electronic energy levels.

2. Mircowave Spectroscopy: 3P

Classification of molecules, rigid rotor model, effect of isotopic substitution on the transition frequencies, intensities, non-rigid rotor. Stark effect, nuclear and electron spin interaction and effect of external field.

Home assignment for students: Applications of Mircowave Spectroscopy.

3. **Vibrational Spectroscopy:** 15P

A. **Infrared Spectroscopy:** Review of linear harmonic oscillator, vibrational energies of diatomic molecules, zero point energy, force constant and bond strengths; an harmonicity, Morse potential energy diagram, vibration-rotation spectroscopy, P, Q, R, branches. Breakdown of Oppenheimer approximation; vibrations of polyatomic molecules. Selection rules, normal modes of vibration group frequencies, overtones, hot bands, factors affecting the band positions and intensities, far IR region, metal-ligand vibrations, normal co-ordinate analysis.

B. **Raman Spectroscopy:** Classical and quantum theories of Raman Effect. Pure rotational, vibrational and vibrational-rotational Raman spectra, selection rules, mutual exclusion principle. Resonance Raman Spectroscopy,

Home assignment for students: Coherent anti Stokes Raman Spectroscopy (CARS.)

4. Electronic Spectroscopy 15P

A. Atomic Spectroscopy: Energies of atomic orbitals, vector representation of momenta and vector coupling, spectra of hydrogen atom and alkali metal atoms.

B. Molecular Spectroscopy: Energy levels, molecular orbitals, vibronic transitions, vibrational progressions and geometry of the excited states, Franck-Condon principle, electronic spectra of polyatomic molecules. Emission spectra; radioactive and non-radioactive decay, internal conversion, spectra of transition metal complexes, charge-transfer spectra.

C. Photoelectron Spectroscopy: Basic principles; photo-electric effect, ionization process, Koopman's theorem.

Home assignment for students: Auger electron spectroscopy -basic idea.

5. Magnetic Resonance Spectroscopy: 20P

A. Nuclear Magnetic Resonance Spectroscopy:

Nuclear spin, nuclear resonance, saturation, shielding of magnetic nuclei, chemical shift and its measurements. Factors influencing chemical shift. Deshielding, spin-spin interactions, factors influencing coupling constant J. Classification (ABX, AMX, ABC, A_2B_2 etc.) spin decoupling; basic ideas about instrument. NMR studies of nuclei other than proton - ^{13}C and ^{19}F. FT NMR, advantages of FT NMR, use of NMR in medical diagnostics.

Home assignment for students: NMR studies of nuclei other than proton - ^{31}P

B. Electron Spin Resonanace Spectroscopy:

Basic principles zero field splitting and Karmer's degeneracy, factors affecting the 'g' value. Isotropic and anisotropic hyperfine coupling constants, spin Hamiltonian, spin densities and McConnell relationship, measurement techniques, applications.

C. Nuclear Quadrupole Resonance Spectroscopy:

Quadrupole nuclei, quadrupole moments, electric field gradient, coupling constant splitting. Applictions.

Books Suggested

1. Modern Spectroscopy - J.M. Hollas, John Wiley
2. Applied Electron Spectroscopy for Chemical Analysis d.H.Windawi & F.L.Wo.Wiley Interscience.
3. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, R.V. Parish, Ellis Harwood.
4. Physical Methods in Chemistry - R.S. Drago, Saunders College.
5. Introduction to molecular Spectroscopy - G.M.Barrow, McGraw Hill.
6. Basic Principles of Spectroscopy - R.Chang, McGraw Hill.
7. Theory and Applications of UV Spectroscopy - H.H.Jaffe & M.Orchin,IBH-Oxford.
8. Introduction to Phoroelectron Spectroscopy - P.K.Ghosh, John Wiley.
9. Introduction to Magentic Resonance - A.Carrington & A.D. Maclachalan, Harper & Row.

Outcomes: Students will be able to:

- Explain the basic principles of rotational, vibrational, electronic and Raman spectroscopy.
- Identify and explain factors that influence the strength and frequency of peaks in the Microwave, IR spectra.
- Describe the selection rule for rotational, Vibrational and electronic spectroscopy.
- Determine the vibrations for a molecule and identify whether they are active in infrared and/or Raman spectroscopy.
- Explain the difference between Stokes and anti-Stokes lines in a Raman spectrum and justify the difference in intensity between Stokes and anti-Stokes lines.
- Draw the Stokes and anti-Stokes lines in a Raman spectrum of a compound when given the energies of the different transitions.
- Understand the electronic spectra of atomic and diatomic molecular systems.
- Justify the absorption lines in atomic electronic spectra and the broad bands in molecular electronic spectra.
- Able to interpret the molecular electronic spectra and deduce the electronic structure information in ground and excited states of diatomic molecules.
- Importance of the Nuclear Quadrupole Resonance Spectroscopy in the characterizing organic and inorganic compounds.
- Know how the electric fields gradient in molecules influences NQR, and ESR spectra.

M. Sc. First Year, Semester-I
Biophysical Chemistry
Paper : X (ECH-421)
Credit - 04

Marks : 75 **60 P**

Objectives :

- Biophysical chemistry basically deals with study of determination and analysis of macromolecular structures and the applications of quantitative methods to analyse biological systems
- This also covers the biochemistry concern with physical and chemical properties of biomacromolecules and its importance in the various functions and forms of various transport processes.

Course Content:

1. **Biological Cell and its Constituent:** **10p**
   Biological cell structure and function of proteins, enzymes, DNA and RNA in living system, helix-coil transition.
2. **Bioenergetics:** **10P**
   Standard free energy change in biochemical reaction, exergonic, enderonic, hydrolysis of ATP, Synthesis of ATP from ADP.
3. **Statistical Mechanics in Biopolymers:** **10P**
   Chain configuration of macromolecules, statistical distribution, end to end dimensions, calculation of average dimension of various chain structures, polypeptide and protein structures, introduction to protein folding problem.
4. **Biopolymer Interactions:** **10P**
   Forces involved in biopolymer interactions, electrostic charges and molecular expansion, hydrophobic forces, dispersion force interactions, multiple equilibria and various types of binding processes in biological systems, hydrogen ion titration curves.
5. **Thermodynamics of Biopolymer Solution:** **10P**
   Thermodynaimcs of biopolymer solutions, osmotic pressure, membrane equilibrium, muscular contraction and energy generation in mechanochemical system.
6. **Cell membrane and transport of ions:** **10P**
   Structure and functions of cell membrane, ion transport through cell membrane, irreversible thermodynamics treatment of membrane transport, nerve conduction.

Book Suggested:

Principles of Biochemistry – by A. LO. Lehniger, Worth Publisher
Biochemistry – by L. Stryer, W. H. Freeman
Biochemistry – by J. Devidrawn, Neil Patterson
Biochemistry – by Veot, John Wiley
Qutines of Biochemistry – by E. E. Conn, P. K. Stumpf, John Wiley

Bioinorganic Chemistry : A Chemical Approach to Enzyme Action – by H. Dugas, C. Penny, Springer – Verlag.
Macromolecules structure and functions – by f. Would, Prentice Hall.

Outcome :

- Students will learn biological organisation of cells, constituents of cell , structure and its functions in the living organisation.
- The biochemical processes such as oxidation, reductions, enzyme catalysis bioenergetics nerve conduction, muscle contraction in the human body are very much important thus the study of chemical basis of life and chemical reactions strengthen the knowledge of Biochemistry also.

M. Sc. First Year,
Laboratory Course – I
(Inorganic Chemistry)
Paper : XI (LCH-411)
Credit - 04

Marks : 75 **120P**

Objectives:

- To understand the role of various factors in structure determination of coordination complexes, the operating procedures and principles lying behind applications of various analytical techniques in determination of structure of complexes.
- To learn the basic principles involved in the analysis of inorganic mixtures such as acidic and basic radicals, sodium carbonate extract, its preparation and use while analysis, original solution, its preparation and use, group reagents, spot test reagents and their use while analyzing inorganic mixture, solubility product, common ion effect etc
- To understand the reactions taking place while analyzing various acidic and basic radicals in a given mixture and to deepen the level of understanding of inorganic chemistry.

1. Record and viva voce 05
2. Detection of three acidic and three basic radicals from a given salt mixture.
   Report the spot test of radicals. (At least five mixtures) 15
3. Preparation of metal complexes and characterized by spectral analysis.
   a. Tris-(thiourea) copper(I) sulphate
   b. Bis (acetylacetanato) copper (II)
   c. Potassium trioxalato ferrate(III)
   d. Cis -potassium dioxalato diaquo chromate(III)
   e. Bis(dimetyl glyoxime) Nickel (0) Complex
   f. Hexammine nickel(II) Chloride
   g. Tris(Acetyl acetanato) Magnease(III)
   i. Schiff's base copper (II) Complexes 15
4. Separation and estimation of one of the metal ion volumetrically.
   a. Fe+3 and Zn+2 b. Ni+2 and Cu+2
   c. Cu+2 and Ba+2 d. Ni+2 and Zn+2
   e. Cu+2 and Fe+2 f. Ba+2 and Mg+2 15

Outcome: Students will be able to

- Learn synthesis methods for the preparation of various coordination complexes and will understand the basic principles involved in operational procedures while synthesizing the complexes to a deeper level.
- To characterize a synthesized complex using various characterization techniques such as melting point determination, solubility behavior in various solvents, molar conductance, magnetic susceptibility measurements, IR and electronic spectra etc.
- While following all these methods he/she will be able to understand operation procedures, care that should be taken while using these techniques and the practical utility of these techniques.
- Understand the basic principles lying behind inorganic analysis such as precipitation, solubility product, buffer solution, applications of buffer solution in maintaining pH, common ion effect etc. and this much information will be helpful while analyzing any inorganic compound in future.

M. Sc. I Semester
Laboratory Course II
(Organic Chemistry)
Paper XII : (LCH - 412)

Marks : 75 **120 P**

Objectives:

- To learn the techniques of separation of organic mixtures
- To apply the skill in two stage preparation
- To adopt skill of purification and crystallization
- To able to understand the estimation of given organic compound
- To understand micro scale technique.

1. Techniques:

a) Simple distillation.
b) Steam distillation.
c) Thin layer chromatography.
d) Column chromatography.

2. Qualitative analysis:

a) Separation, Purification, sample submission and identification of compounds of binary
mixture (one solid and one liquid) by chemical method (Any six).
b) Separation, Purification, sample submission and identification of compounds of binary mixture (solids) physical method (Any three).

3. Preparations (Double stage), (Any Four):

a) Phthallic anhydride-phthalimide-Anthranilic acid.
b) Acetophenone-oxime-Acetanilide.
c) Phthallic anhydride-o-benzoyl benzoic acid-Anthraquinone.
d) Chlorobenzene-2,4-dinitrochlorobenzene-2,4-dinitrophenol.
e) Benzoin-benzil-benzilic acid.
f) Acetanilide-p-bromoacetanilide-p-bromo aniline.

4. Use of Computer (ChemDraw, ChemSketch, ISI Draw):

Draw the structure of aliphatic, aromatic and heterocyclic compounds and get the correct IUPAC name.

Reference Book:

1. Vogel practical organic chemistry.

Outcomes : Students will be able to

- Learn the pilot separation of the binary mixture
- Familiarize the systematic procedure of organic mixture analysis
- The preparation involving nitration, bromination, Sandmayer reaction, and Aldol condensation
- Learn the test involving identification of special elements
- Learn the confirmatory test for various functional groups
- Understand the technique involving drying and crystallization by various methods
- Expertise the various techniques of preparation and analysis of organic substances
- Learn the estimation of various organic compounds.
- Understand micro scale technique.

M. Sc. I Semester
Laboratory Course III
(Physical Chemistry)
Paper XIII : (LCH - 413)

Marks : 75 **120 P**

Objective:

- To understand basic principles and theory of different instruments
- To perform different experiments on conductometer, pH meter, potentiometer, calorimeter, polarimeter, refractometer.

N.B. 1. Performance of eighteen experiments is expected
2. At least one experiment on each instrument should be done.
3. Student should prepare the required solutions

SECTION - A

INSTRUMENTATION:

1. CONDUCTOMETER:

1. To estimate the concentrations of sulphuric acid, acetic acid and copper sulphate in given solution.
2. To determine solubility product and thermodynamic properties (ΔG , ΔH, ΔS) of sparingly soluble salts.
3. To determine the relative strength of chloroacetic acid and acetic acid.
4. To determine the hydrolysis constant of Aniline hydrochloride.
5. To investigate basic hydrolysis of ethyl acetate at four different temperatures and to find out the energy of activation .

2. POTENTIOMETER:

1. To determine PK**1** PK**2** values of Phosphoric acid.
2. To determine strength of strong acid and weak acid in given mixture.
3. To determine the oxidation state of metal ion by method of concentration cell without transparence.

3. pH-METER:

1. To determine Hammet constant of given substituted benzoic acid.
2. To determine pH values of various mixtures of sodium acetate and acetic acid in aqueous solution and hence to find out dissociation constant of acid.

4. COLORIMETER

1. To determine equilibrium quotient for formation of mono thiocyanate iron(III) complex.
2. To determine Indicator constant of an indicator.
3. To determine concentration of Cu(II) iron in given solution titrating with E.D.T.A. solution.

5. REFRACTOMETER:

1. To determine the molar refractivity of methyl acetate, ethyl acetate, n-hexane and carbon tetra chloride and to calculate refractive equivalence of C, H and Cl atom.
2. To study the variation of refractive index with composition of mixture of CCl_4 and ethyl acetate.

6. POLARIMETER.

1. To determine the relative strength of two acids.
2. To determine the percentage of two optically active substance (d-glucose and dtartaric acid) in the mixture.

SECTION B

NON-INSTRUMENTATION

1. To determine partial molar volume of ethanol and water mixture at given Composition .
2. To determine molecular weight of high polymer by viscosity measurement.
3. To study the effect of surfactant on surface tension of water by using stalagmometer.
4. To determine solubility of benzoic acid at different temperature and hence to determine it's heat of solution.
5. To investigate the autocatalytic reaction between KMnO4 and oxalic acid and to find energy of activation.
6. To determine the rate constant of hydrolysis of methyl acetate catalyzed by HCl.
7. To determine effect of ionic strength on rate constant of reaction between potassium per sulphate and potassium iodide.
8. To investigate the solubility of three component system and hence tie line on binodal curve.
9. To study the variation of viscosity with composition of mixture of i) ethanol-water ii) methanol-ethylidene chloride iii) nitric acid- Chloroform and determine whether or not there is compound formation between two liquids.
10. To determine surface tension of methyl acetate, ethyl acetate and chloroform and hence to calculate atomic parachors of C, H, Cl.
11. To determine order of reaction of given reaction kinetics by fractional change method.
12. To study distribution of benzoic acid between benzene and water at room temperature and hence show that benzoic acid dimerises in benzene.

Outcome: Student will be able to

- Apply their knowledge for setting various experiments based on the instrumentations studied
- Perform different qualitative and quantitative analysis.

M. Sc. I Semester
Laboratory Course – IV
(Analytical Chemistry)
Paper XIV : (LCH - 414)

Marks : 75 **120 P**

Objective:

- To understand basic principles and theory of different instruments
- To perform different experiments on conductometer, pH meter, potentiometer, calorimeter, polarimeter, refractometer
- To set various experiments based on the different instrumentations
- To understand basic principles and theory of measurements of density, viscosity, refractive index, surface tension, adsorption
- To perform different qualitative and quantitative analysis.

Section-A
(Intrumental)

A. Conductometry

1. Determination of the strength of strong acid and weak acid from mixture solution conductometrically
2. Analysis of aspirin by conductometric method.

B. Potentiometry

1. Determination of the strength of halides in the given mixture using Potentiometry.
2. Determine the acid and basic dissociation constant of an amino acid (Glycine) and hence isoelectric point of an acid

C. pH-metry

1. Acid-base titration in non-aqueous media by pH-metry (benzoic acid in ethanol / NaOH).
2. Determination of pKa of weak acid by pH-metry.
3. Determination of degree of dissociation of weak electrolyte and to study the deviation from ideal behaviour that occurs with a strong electrolyte.

D. **Colorimetry**

1. Varification of Beer's law for a) $KMn0_4$ and Cu^{+2} ammonia complex solution.
2. Determination of empirical formula for the formation of ferric salicylate complex by Job's method.
3. Determination of stability constant for the formation of complex between Fe^{3+} ions and 5-sulphosalicylic acid.

E. Polarimetry

1. Determination of rate constant for inversion of cane sugar by polarimetry.
2. Study of inversion of cane sugar by enzyme kinetics.
3. **D**etermine the percentage of two optically active substances in a mixture polarimetrically.

F. Flame photometry

1. Estimation of Na^+ / K^+ by Flame photometry.

Section-B

(Non-Instrumental)

A. Statistical analysis

1. Application of **'t'** test for experimental data.
2. Application of rejection criteria (Q test) for experimental data.
3. Treatment of analytical data with least square method applied to Beer's law for $KMn0_4$ solutions.

B. Chromatography

1. Separation of cations and anions by paper chromatography and determination of Rf values.
2. Determination of Ion-exchange capacity of an cation exchanger.
3. Determination of Ion-exchange capacity of an anion exchanger.

C. Chemical Kinetics

1. Investigate the reaction between bromic acid and hydroiodic acid.
2. To study the kinetics of iodination of acetone.

D. Heterogeneous equilibria:

1. Determine the formula of complex form between Cupric ion and ammonia by distribution method.
2. Investigate the solubility of three component system and hence draw a tie lone on bimodal curve.
3. Determination of hardness of water by complexometric titration.

Outcome: Student will be able to

- Understand the basic principles and theory of different instruments used during the conduction of the experiments
- Perform the different experiments on conductometer, pH meter, potentiometer, colorimeter, polarimeter, flame photometry
- Apply their knowledge for setting various experiments based on the instrumentations studied
- Perform different qualitative and quantitative analysis.