GANDHI INSTITUTE OF TECHNOLOGY AND MANAGEMENT (GITAM)
(Deemed to be University)
VISAKHAPATNAM * HYDERABAD * BENGALURU

Accredited by NAAC with A^+ Grade

CURRICULUM AND SYLLABUS

of

Master of Science

in

CHEMISTRY (PHARMACEUTICAL CHEMISTRY as Specialisation)

(for 2022-23 admitted batch)

Program Educational Objective (PEOs), PO's (Program Outcomes), and PSO's (Program Specific Outcomes)

Program Educational Objective (PEOs)

The PEOs are broad statements that describe the career and professional accomplishments that the program is preparing its graduates to achieve in few years (for example two years) subsequent to receive the degree. The PEOs of the M.Sc. program in Chemistry are as follows:

PEO 1: GU Chemistry graduates will be well prepared for successful careers in the profession or in research & innovation at an industry and/or in government in one or more of discipline of chemistry and /or sub disciplines of Chemistry.

PEO 2: GU Chemistry graduates will be academically prepared to provide feasible and sustainable solutions for real-life problems and become licensed professional chemists in due course and will contribute effectively in serving the society.

PEO 3: GU Chemistry graduates will be engaged in professional activities to enhance their own achievement and simultaneously contribute in service of humankind.

PEO 4: GU Chemistry graduates will be successful in higher education in Chemistry and in management, if pursued.

PEO 5: GU Chemistry graduates will be successful leaders with quality to handle all kind of diverse circumstances through nurturing them in interdisciplinary and multidisciplinary learning environment.

PO's (Program Outcomes)

Program Outcomes (POs) are attributes of the graduates that describe the professional career accomplishments that the programs designed.

Outcomes:
PO 1: Apply knowledge of Chemistry and chemistry specializations to solution of complex scientific problems. *(Scientific knowledge)*

PO 2: Identify, formulate, research literature, and analyze complex scientific problems reaching substantiated conclusions using principles of chemistry. *(Problem analysis)*

PO 3: Design of solutions for complex scientific problems and design of chemical processes that meet the specified needs with appropriate considerations of public health and safety, and cultural, societal, and environmental considerations *(Design/development of solutions)*

PO 4: Use research based methods including design of experiments, analysis and interpretation of data and synthesis of chemical products leading to logical conclusions *(Conduct investigations of complex problems)*

PO 5: Create, select, and apply appropriate techniques, resources, and modern scientific and IT tools including prediction and modelling complex scientific activities with an understanding of limitations *(Modern tool usage)*

PO 6: Apply reasoning within the contextual knowledge to access societal, health, safety, legal, and cultural issues and the con-sequent responsibilities relevant to the professional scientific practice *(The chemist and society)*

PO 7: Understand the impact of the professional scientific solutions in the societal and environmental contexts, and demonstrate the knowledge of, and the need for sustainable developments *(Environment and sustainability)*

PO 8: Apply ethical principles and commit to professional ethics and responsibilities and norms of scientific practice *(Ethics)*

PO 9: Function effectively as an individual independently and as a member or leader in diverse teams, and in multidisciplinary settings *(Individual and team work)*

PO 10: Communicate effectively on complex scientific activities with the science community and with society at large such give and receive clear instructions *(Communication)*

PO 11: Demonstrate knowledge and understanding of scientific management principles and apply those to one's own work as a member and leader of a team to manage projects in multidisciplinary environments *(Project management and finance)*

PO 12: Recognize the need for, and have the preparation and ability to engage in independent and life-long learning in the broadest context of technological change *(Life-long Learning).*

Program Specific Outcomes (PSOs)

Program Specific Objectives (PSOs) are specific statements that describe the professional career accomplishments that the programs designed. The PSOs of the M.Sc. Program in Chemistry are program are as follows:

PSO 1: Chemistry graduates will be prepared to contribute effectively in the areas of organic chemistry and able to apply the concept of advance studies for the understanding of underlining principles, proposing mechanism, problem solving, identification of chemical species and arriving to logical conclusion by developing skills in synthesis and characterization of specific organic compounds using documented laboratory procedures.

PSO 2: GU Chemistry graduates will be able to integrate knowledge learned in different courses of Inorganic and Environmental Chemistry. This learning will help students to meet the demands of various Industries based on chemicals as well as environmental science. And students will also utilize this knowledge to handle all types of hazardous and toxic chemicals along with all necessary required precautions.

PSO 3: GU Chemistry graduates will be able to acquire firm knowledge over various fundamental theories related with Physical and Analytical Chemistry. By using concepts, tools and techniques related to these topics, they can acquire knowledge and utilize its application in interpretation and explanation of the limits, accuracy of experimental data in terms of significance.

M.Sc. CHEMISTRY (PHARMACEUTICAL) - I SEMESTER

SCY 701: COORDINATION CHEMISTRY

Hours per week	: 4	Semester End Examination	: 60 Marks
Credits	: 4	Continuous Evaluation	: 40 marks

Preamble

This course is designed to explain the students about bonding in coordination compounds, magnetic properties and colour of coordination compounds, basic spectroscopic properties of compounds, stability of metal complexes in solutions and mechanisms of ligand substitution and electron transfers in coordination complexes

Course objectives:

- To obtain an introductory knowledge of bonding in coordination compounds
- To understand the magnetic properties and colour of coordination compounds
- To understand the basic spectroscopic properties of compounds
- To acquire a knowledge in stability of metal complexes in solutions
- To obtain a detailed knowledge in mechanisms of ligand substitution and electron transfers in coordination complexes

UNIT-I

Metal-ligand bonding: Crystal field theory - crystal field splitting patterns in octahedral,tetrahedral tetragonal, square planar, square pyramidal and trigonal bipyramidal geometries-Determination of crystal field splitting energy - calculation of crystal field stabilization energies - Factors affecting crystal field splitting energies- spectrochemical series - MLCT and LMCT transitions in coordination compounds - Jahn-Teller effect –Molecular Orbital theory - ligand field theory.

Learning Outcomes*:*

By the end of this unit, the student will able to

- Understand the bonding and structures of complex compounds (**L1**)
- Learn how to calculate the crystal field energies (**L3**)

UNIT-II

Electronic spectra: Term symbols - Russell–Saunders coupling - derivation of term symbolsfor various configurations. Spectroscopic ground states, selection rules, correlation diagrams - Orgel and Tanabe-Sugano diagrams for transition metal complexes (d^1-d^9 states), calculations of Dq, B and β parameters, charge transfer spectra.

Learning Outcomes*:*

By the end of this unit, the student will able to

- Understand the spectroscopic properties of compounds (**L1**)
- Predict the suitable method to characterize the inorganic compounds by Mossbauer (**L2**)

UNIT-III

Metal-Ligand Equilibria in solutions: Stepwise and overall formation constants and theirinteraction,Trends in successive formation constants, factors effecting the stability of metal

complexes with reference to the nature of metal ion and ligand, the chelate effect, determination of formation constants by pH metry and spectrophotometry. The Irving-Williams series.

Learning Outcomes*:*

By the end of this unit, the student will able to

- Lean the solution chemistry principles (**L1**)
- Understand the influence of metal and ligand on stabilization of complexes (**L3**)

UNIT-IV

Mechanisms of Inorganic Reactions-I: Energy profile of a reaction, reactivity of metalcomplexes, inert and labile complexes, Substitution reactions in octahedral complexes-kinetics of octahedral substitution, acid hydrolysis, factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism, anation reactions, reactions without metal ligand bond cleavage. Substitution reactions in square planar complexes, the trans effect in Pt(II) complexes, Polarisation and π-bonding theories of trans effect.

***Learning Outcomes**:*

By the end of this unit, the student will able to

- Lean the reactivity and kinetics of coordination complexes (**L1**)
- Analyze the various types of substitution reactions (**L3**)

UNIT-V

Mechanisms of Inorganic Reactions-II: Oxidation-reduction reactions, classification of redoxreactions, mechanism of one electron transfer reactions, Inner sphere redox reactions, outer sphere redox reactions, mixed inner and outer sphere reactions, two equivalent-one equivalent reactions of thallium(III)-thallium(I) and Hg(I)-Hg(II).

***Learning Outcomes**:*

By the end of this unit, the student will able to

- Lean the kinetics in electron transfer reactions of coordination complexes (**L2**)
- Distinguish between ligand transfer and electron transfer reactions (**L3**)

Course outcomes:

After the completion of the course, the student will be able to

Acquire knowledge about the structure and bonding in coordination compounds, CFT theory and application of CFT in real life (L1)

Understand the spectroscopic properties of compounds and parameters. Principles of Mossbaur spectroscopy and applications (L2)

Learn the principles of solution chemistry (L3)

Explain the reactivity of metal complexes and substitution reactions (L4)

List the electron transfer reactions and knowing the mechanism of transfer reactions (L5)

Text Books

1) Advanced Inorganic Chemistry by F.A.Cotton and R.Wilkinson, VI Edition, Johnwilly and sons, New York, 2007.
2) Inorganic Chemistry: Principles of Structure and Reactivity by James E. Huheey, Okhil K. Medhi Ellen A. Keiter, Richard L. Keiter, 2006.
3) Inorganic Chemistry, Gary L. Miessler and D. A. Tarr, 3rd Edition 2004, Pearson-Prentice Hall.
4) Mechanisms of Inorganic Reactions in solution by D.Benson, McGraw Hill, London, l968.
5) Mechanisms of Inorganic reactions: A study of metal complexes in solutions, F. Basalo& R. G. Pearson, Wieley-Eastern Pvt Ltd., 2ndEdn.
6) Kinetics and Mechanisms of reactions of Transition metal complexes by Ralph G. Wilkins, Wieley-VCH, Verlog GmbH & Co., 2002

	Program Objectives(POs)												PSOs		
	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**	**1**	**2**	**3**
CO1	2	3	1	1	1	3	1	1	1	1	2	3	1	3	1
CO2	2	3	2	3	2	3	1	1	2	2	2	2	1	2	3
CO3	3	2	3	1	2	2	2	1	3	1	1	3	2	1	3
CO4	2	2	3	2	3	2	1	2	1	1	1	2	1	3	2
CO5	2	3	2	2	1	2	2	2	1	1	1	3	1	3	2

SCY 703: CONCEPTS OF ORGANIC CHEMISTRY

Hours per week	: 4	Semester End Examination	: 60 Marks
Credits	: 4	Continuous Evaluation	: 40 marks

Preamble

This course is designed to explain the students about Nature of bonding in Organic Molecules, reactive intermediates; Stereochemistry and Stereoisomerism; Addition Mechanisms; various rearrangements; importance of some Natural Products

Course Objectives:

- To explain Nature of bonding in Organic Molecules, Concept of aromaticity, types of organic reactions and reactive intermediates.
- To explain Stereochemistry and Stereoisomerism:Conformational/Optical/geometrical isomerism.
- To explain Additionto carbon-carbon multiple bonds orientation and stereochemistry.
- To explain various rearrangements:general mechanistic treatment to rearrangements.
- To explain Isolation, structure elucidation and synthesis of some important Natural Products.

UNIT- I

Nature of bonding in Organic Molecules: Localised and delocalised covalent bond, concept ofaromaticity annulenes and hetero annulenes, inductive and mesomeric effects. Huckel‟s rule for aromaticity in benzenoid and non-benzenoid compounds, anti-aromaticity and homo-aromaticity. Introduction to types of organic reactions and reactive intermediates.

Learning Outcome

At the end of the unit, the student will be able to understand:

- Inductive, mesomeric effects in organic molecules **(L1)**
- Aromaticity,homo/anti-aromaticity in various benzenoid and non-benzenoid systems **(L2)**
- Types of organic reactions **(L3)**
- Reactivity and stability ofreactive intermediates **(L4)**

UNIT- II

Stereochemistry and Stereoisomerism: Conformational isomerism and analysis in acyclic andsimple cyclic systems - substituted ethanes, cyclopentane, cyclohexane, cycloheptane, cyclo octane and decalins. Optical isomerism - optical activity -molecular dissymmetry and chirality (Chiral centre, chiral axis, chiral plane), elements of symmetry. Fisher's projection D,L. and R,S. configurations - relative and absolute configurations, optical isomerism due to asymmetric carbon atoms, optical isomerism in biphenyls, allenes and spirans. Optical isomerism of nitrogenous compounds, racemisation and resolution - geometrical isomerism and E,Z configurations, properties of geometrical isomers. Recognition of symmetry elements and chiral structures, R-S-nomenclature, diastereoisomerism in acylic and cyclic systems inter conversions of Fisher, Newman and Saw-horse projections.

Learning Outcome

At the end of the unit, the student will be able to learn

- Conformational isomerism, analysisin acyclic and simple cyclic systems **(L1)**

- D,L. and R,S. configurations,Optical isomerism (**L2**)
- E,Z configurations,R-S-nomenclature (**L3**)
- Fisher, Newman and Saw-horse projections (**L4**)

UNIT- III

Addition Mechanisms: Addition to carbon-carbon multiple bonds. Addition reactions involvingelectrophiles, nucleophiles and free radicals, cyclic mechanisms, orientation and stereochemistry.

Learning Outcome

At the end of the unit, the student will be able to learnaboutAddition Mechanisms of

- Carbon-carbon multiple bonds involving (**L1**)
- Electrophiles (**L2**)
- Nucleophiles (**L3**)
- Free radicals, and their rules (**L4**)

UNIT- IV

Rearrangements: Classification and general mechanistic treatment of nucleophilic, free radicaland electrophilic rearrangements, Wagner–Meerwein, Tiffeneau–Demjanov rearrangement, Neber, Hofmann, Stevens ,Wittig and Fries rearrangements.

Learning Outcome

At the end of the unit, the student will be able to learn **the** Mechanisms of rearrangement

- Wagner–Meerwein (**L1**)
- Tiffeneau–Demjanov (**L2**)
- Neber, Hofmann (**L3**)
- Stevens ,Wittig and Fries rearrangements (**L4**)

UNIT- V

Natural Products: Isolation, structure elucidation and synthesis of alkaloids: atropine, nicotine,papaverine, purines: caffeine. flavonoids: quercetin: genestein. terpenoids: citral ,α-terpeneol, camphor.

Learning Outcome

At the end of the unit, the student will be able to know the importance of

- Alkaloids: atropine, nicotine, papaverine (**L1**)
- Purines: caffeine (**L2**)
- Flavonoids: quercetin, genestein (**L3**)
- Terpenoids: citral ,α- terpeneol, camphor (**L4**)

Textbooks:

1. Organic Chemistry, Vol. I (Sixth Edn), and Vol. II (Fifth Ed.), by I.L.Finar, ELBS, 2002
2. Organic Chemistry (Fifth Edn.)by Morrison and Boyd, PHI, India, 2011
3. Organic Chemistry by Mukhergee, Singh and Kapoor, Vols, I and II, Wiley Eastern., 2010
4. Reaction Mechanism in Organic Chemistry by Mukherjee and Singh, Macmillan India., 2012
5. A guide book to mechanism in Organic Chemistry by Peter Sykes, ELBNS., 1986
6. Advanced Organic Chemistry by Jagdamba Singh and L D S Yadav,Pragati Edition., 2010
7. Organic reactions, Stereochemistry, and Mechanism, P.S. Kalasi, New Age International,2007

Reference Books:

1. Advanced Organic Chemistry by Jerry March (3rd Edn.) Wiley Eastern, 2006
2. Stereochemistry of carbon compounds by E.Eliel. McGraw Hill., 2008

Course outcomes:
After the completion of the course, the student will be able to

- **Describe** inductive, mesomeric effects in organic molecules and reactivitiy and stability of reactive intermediates aromaticity,homo/anti-aromaticity in various benzenoid and non-benzenoid systems (**L1)**
- **Understand** the concepts of Geometrical Isomerism, Relative (D, L) and Absolute (R, S) configurations, Optical isomerism and Conformational Isomerism (**L2)**
- **Teach** the addition Mechanisms of carbon-carbon multiple bonds involving electrophiles, nucleophiles, free radicals, and their rules (**L3)**
- **Illustrate** mechanisms of rearrangement like Wagner–Meerwein, Tiffeneau–Demjanov, Neber, Hofmann, Stevens, Wittig and Fries rearrangements (**L4)**
- **Evaluate** the importance of alkaloids like atropine, nicotine, papaverine, purines like caffeine, flavonoids like quercetin, genestein; terpenoids like citral ,α- terpeneol, camphor (**L5)**

	Program Objectives(POs)												**PSOs**		
	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**	**1**	**2**	**3**
CO1	1	2	1	1	2	3	2	3	2	2	2	3	3	2	3
CO2	2	1	3	2	2	1	3	2	2	1	3	2	1	3	2
CO3	1	3	1	2	1	3	1	2	1	3	1	2	3	1	2
CO4	1	1	2	1	1	1	2	1	1	1	2	1	1	2	1
CO5	3	2	1	3	3	2	1	3	3	2	1	3	2	1	3

1-Low, 2- Medium and 3- High Correlation

SCY 705: CHEMICAL KINETICS AND THERMODYNAMICS

Hours per week	: 4	Semester End Examination	: 60 Marks
Credits	: 4	Continuous Evaluation	: 40 marks

Preamble

Chemical kinetics explains about theories Arrhenious, reaction coordinates transition state, thermodynamic formulation of reaction rates. It emphasis on Reactions in solution- primary and secondary salt effects, effect of solvent on reaction rate; effect of substituents on reaction rates. Thermodynamics describes macroscopic behavior of a system in a time-invariant state in terms of bulk properties such as pressure, volume, temperature and chemical potential. It is also concerned with the potential functions obtained by combining these properties and their relation to spontaneity of physical and chemical processes.

Course Objectives

- To provide insights into the concept of Collision theory, Arrhenious equation.
- To introduce the idea of Unimolecular reactions- Lindemann's theory and RRKM theory.
- To demonstrate the laws of thermodynamics through real-life examples and applications.
- To generate an intuitive understanding among the students for the concept of entropy and its relevance in design of a heat engine.
- To demonstrate how thermodynamics dictates the feasibility of physical transformations and chemical reactions.

Chemical Kinetics

UNIT –I

Theories of reaction rates- Collision theory, Steric factor; Theory of absolute reaction rates- Reaction coordinate, transition state, thermodynamic formulation of reaction rates; Unimolecular reactions- Lindemann‟s theory and RRKM theory; **Reactions in solution**- primary and secondary salt effects, effect of solvent on reaction rate; effect of substituent‟s on reaction rate - Hammett and Taft equations with examples - Linear Free Energy relations

Learning Outcomes:

By the end of this Unit, the student will be able to understand

- Theories of reaction rates, collision theory, transition state theory. (**L1**)
- Thermodynamic formulation of reaction rates, Reactions in solution- primary and secondary salt effects, effect of solvent on reaction rate. (**L2**)
- Hamett and Taft equations with examples - Linear Free Energy relations. (**L3**)

UNIT –II

Catalysis: Homogeneous catalysis- acid-base catalysis- mechanism of acid-base catalysis - Enzyme catalysis- Michaelis-Menten kinetics - Heterogeneous catalysis- Langmuir adsorption

isotherm- unimolecular and bimolecular reactions-catalytic poisoning-active centers, surface area-determination of surface area with BET equation.

Learning Outcomes:

By the end of this Unit, the student will be able to understand

- Homogeneous catalysis- acid-base catalysis- mechanism of acid-basecatalysis - Enzyme catalysis. (**L1**)
- Unimolecular and bimolecular reactions-catalytic poisoning-active centers. (**L2**)

UNIT –III

Complex reactions: Opposing, parallel and consecutive reactions (all first order type)-derivation of rate-law, Chain reactions- derivation of rate-laws for H_2-Cl_2 and H_2-Br_2 reactions; Fast reactions-study of fast reactions by flow methods and relaxation methods

Learning Outcomes:

By the end of this Unit, the student will be able to understand

- Opposing, parallel and consecutive reactions. (**L1**)
- Chain reactions- derivation of rate-laws for H_2-Cl_2 and H_2-Br_2 reactions. (**L2**)
- Fast reactions-study of fast reactions by flow methods and relaxation methods. (**L3**)

UNIT –IV

Thermodynamics: Second law of thermodynamics- concept of entropy-entropy change in reversible process andirreversible process-entropy of mixing; Fugacity: concept-Determination-Variation of fugacity with pressure; concept of partial molar properties- chemical potential-significance-variation with preassure and temperature- Gibbs-Duhem equation; Van‟t Hoff reaction isotherm, Claussius-Claperyon equation

Learning Outcomes:

By the end of this Unit, the student will be able to understand

- Concept of entropy-entropy change in reversibleprocess and irreversible process. (**L1**)
- Fugacity: concept-Determination- Variation of fugacity with pressure; concept of partial molar properties- chemical potential. (**L2**)
- Gibbs-Duhem equation; Van’t Hoff reaction isotherm, Claussius-Claperyon equation.

(**L3**)

UNIT –V

Third law of thermodynamics- Nernst heat theorem-determination of absolute entropy-limitations of third law of thermodynamics; Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac statistics, Partition function-rotational, translational, vibrational and electronic partition functions for diatomic molecules.

Learning Outcomes:

By the end of this Unit, the student will be able to understand

- Nernst heat theorem-determination of absoluteentropy-limitations of third law of thermodynamics. (**L1**)
- Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac statistics. (**L2**)
- Partition function-rotational, translational, vibrational and electronic partition functions for diatomic molecules. (**L3**)

Course Outcomes

At the end of the unit, the student will be able to

- **Understand** theories on collision theory, transition state theory primary and secondary salt effects, effect of solvent on reaction rate, Linear Free Energy relation (**L2)**
- **Identify** the kinetics studies of Homogeneous catalysis- acid-base catalysis- mechanism of acid-basecatalysis - Enzyme catalysis, Unimolecular and bimolecular reactions-catalytic poisoning-active centers (**L3)**

- **Distinguish** the rate laws of complex reactions ofOpposing, parallel,consecutive reaction and chain reactions- H_2-Cl_2 and H_2-Br_2 reactions as well as methods of study of fast reactions (**L4**)
- **Illustrate** the concept of entropy-entropy change in reversibleprocess and irreversible process. Fugacity: concept of partial molar properties- chemical potential.Gibbs-Duhem equation; Van't Hoff reaction isotherm, Claussius-Claperyon equation. **(L2)**
- **Interpret** the relations of Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac statistics.Partition function-rotational, translational, vibrational and electronic partition functions for diatomic molecules (**L5)**

	Program Objectives(POs)												**PSOs**		
	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**	**1**	**2**	**3**
CO1	2	2	1	3	2	3	2	3	2	2	2	3	3	2	3
CO2	2	1	3	2	2	1	3	2	2	3	3	2	1	3	2
CO3	1	3	2	2	1	2	1	2	1	3	1	3	3	1	2
CO4	1	1	2	1	1	1	2	1	1	1	2	1	1	3	1
CO5	2	2	1	3	3	2	1	3	3	2	1	3	2	1	3

Text Books:

1. Chemical Kinetics, K. J. Laidler, 3rd. Ed, Pearson education (Singapore) Pte. Ltd., New Delhi, 2004
2. Kinetics and Mechanism of Chemical Transformations, J. Rajaraman and J. Kuriacose, McMillan India, 1993
3. A text book of Physical Chemistry, 3rd edition, Vol. 2,3 and 5, K.L.Kapoor, Macmillan, India Limited, 2012
4. Physical Chemistry – P. W. Atkins, Oxford University press, VIIth edition,2002.
5. Thermodynamics A Core Course- R. C. Srivastava, S. K. Saha and A. K. Jain, Prentice-Hall of India, II Edition, 2004.

SCY 707: MOLECULAR SPECTROSCOPY

Hours per week	: 4	Semester End Examination	: 60 Marks
Credits	: 4	Continuous Evaluation	: 40 marks

Preamble

Molecular spectroscopy explains the definition of electromagnetic radiation, different regions of spectrum, polarization of light; plane of vibration, plane of polarization, optical activity, factors effecting the angle of rotation, specific rotation, optical rotator dispersion and circular dichroism, cotton effect. It emphasis on Vibrational and rotational Spectroscopy, Raman effect-Classical and quantum mechanical explanations, Electronic spectra of diatomic molecules- vibrational course structure- intensity of spectral lines- Franck-Condon principle. It deals with the basic ideas about instrument, use of NMR in medical diagnostics,advantages of FT NMR, and Basic principles of ESR, zero field splitting-factors affecting the 'g' value.

Course Objectives

- To provide insights of Electromagnetic radiation- interaction ofelectromagnetic radiation with matter.
- To explain Rotational spectra of diatomicmolecules- rigid rotor-selection rules- calculation of bond length.
- To gain knowledge on position and intensity of spectral lines in Raman and electronic spectra.
- To describe the chemical shift and its measurements, factor influencing chemical shift, deshielding, spin-spin interaction.
- To understand basic principles, zero field splitting-factors affecting the 'g' value.

UNIT-I

Spectroscopy-Unifying Principles: Electromagnetic radiation- interaction of electromagneticradiation with matter- absorption, emission, transmission, reflection, refraction, dispersion and scattering Polarization:polarization of light; plane of vibration,plane of polarization, optical activity, factors effecting the angle of rotation,specific rotation,optical rotator dispersion and circular dichroism, cotton effect

Learning Outcomes:

By the end of this Unit, the student will be able to

- **Understand** the definition of electromagnetic radiation and interaction of electromagnetic radiation with matter **(L1)**
- **Explain** the factors effecting angle of rotation, specific rotation, optical rotator dispersion and circular dichroism, cotton effect **(L2)**

UNIT-II

Vibrational and rotational Spectroscopy : Rotational spectra of diatomic molecules- rigidrotor-selection rules- calculation of bond length- isotopic effect- second order stark effect and its applications, infrared spectra of diatomic molecules-harmonic and anharmonic oscillators-Selection rules- overtones-combination bands-calculation of force constant-anharmonicity constant and Zero point energy . Fermi resonance, simultaneous vibration-rotation spectra of diatomic molecules

Learning Outcomes:

By the end of this Unit, the student will be able to

- **Explain** the rotational spectra of diatomic molecules, rigid rotor-selection rules **(L2)**
- **Understand the s**econd order stark effect and its applications **(L3)**
- **Differentiate** between infrared spectra of diatomic molecules - harmonic and anharmonic oscillators **(L4)**

UNIT-III

Raman Spectroscopy: Raman effect-Classical and quantum mechanical explanations- purerotational, vibrational and vibrational-rotational Raman spectra- selection rules, mutual exclusion principle.

Electronic Spectroscopy: Electronic spectra of diatomic molecules- vibrational course structure-intensity of spectral lines- Franck-Condon principle –applications- rotational fine structure –band head and band shading- charge transfer spectra.

Learning Outcomes:

By the end of this Unit, the student will be able to

- **Understand** the Raman effect, classical and quantum mechanical explanations- pure rotational, vibrational and vibrational-rotational Raman spectra **(L1)**
- **Explain** the electronic spectra of diatomic molecules- vibrational course structure-intensity of spectral lines- Franck-Condon principle – applications (**L2)**

UNIT-IV

Nuclear Magnetic Resonance Spectroscopy: Nuclear spin, nuclear resonance, saturation,shielding of magnetic nuclei, chemical shift and its measurements, factor influencing chemical shift, deshielding, spin-spin interaction, factor influencing coupling constant „J". spin decoupling, basic ideas about instrument, use of NMR in medical diagnostics,advantages of FT NMR.

Learning Outcomes:

By the end of this Unit, the student will be able to

- **Understand** nuclear spin, nuclear resonance, saturation, shielding of magnetic nuclei, chemical shift and its measurements **(L2)**
- **Explain** the factors influencing coupling constant 'J'. Spin decoupling, basic ideas about instrument **(L2)**
- **Illustrate** the use of NMR in medical diagnostics and advantages of FT NMR **(L4)**

UNIT-V

Electron Spin Resonance Spectroscopy: Basic principles, zero field splitting- factors affectingthe „g" value. Isotropic and anisotropic hyperfine coupling constants- experimental technique - applications of ESR studies:deuterium,methyl free radical,benzene free radical,parabenzo semi quinine,copper phthalo cyanine,chloroform,hemoglobin, glycene and alanine.

Learning Outcomes:

By the end of this Unit, the student will be able to

- **Explain** the basic principles of ESR zero field splitting and factors affecting the 'g' value **(L2)**
- **Understand** the experimental technique and applications of ESR. **(L3)**

Course Outcomes

After the completion of the course, the student will be able to

- Categorize the interactions of electromagnetic radiation with matter and interaction of polarized light with different molecules (**L4**)
- Summarize explain the rotational and vibrational energy levels and spectra of diatomic molecules (**L2**)
- Explain the Raman spectra and principle of electronic spectroscopy (**L2**)

- Apply the knowledge of nuclear magnetic resonance spectroscopy in characterizing the molecules and also their use in medical diagnostics (**L3**)
- List out the conditions to observe fine structure of ESR absorption and hyperfine structure (**L4**)

Text Books:

1. C.N. Banwell and E.M. Mc Cash, Fundamentals of Molecular Spectroscopy, 4th edition (1994), Tata McGraw Hill, New Delhi.
2. Introduction to Molecular Spectroscopy, G.M. Barrow, McGraw Hill, 1962
3. Instrumental Methods of Chemical Analysis, Willard, Meritt, Dean & Settle(Wiley Eastern), 7th Ed., 1988

SCY 721: PHARMACEUTICAL CHEMISTRY LAB

Hours per week	: 9	Semester End Examination	: 60 Marks
Credits	: 3	Continuous Evaluation	: 40 marks

1) Organic laboratory techniques, synthesis of organic compounds involving 2 stages.
2) Systematic identification of about six compounds containing one or two functional groups by chemical reactions

SCY 723: PHYSICAL CHEMISTRY LAB

Hours per week	: 9	Semester End Examination	: 60 Marks
Credits	: 3	Continuous Evaluation	: 40 marks

1. Critical solution temperature of phenol -water system
2. Effect of electrolyte (NaCl) on miscibility temperature
3. Comparison of acid strengths through acid catalyzed methyl acetate hydrolysis
4. Conductometric titration of a strong acid with strong base
5. Conductometric titration of a weak acid with strong base
6. Conductometric titration of a mixture of weak and strong acid with strong base
7. Distribution coefficient of I_2 between two immiscible solvents.
8. Equilibrium constant of $KI + I_2 \leftrightarrow KI_3$ by distribution method
9. Potentiometric titration of redox system (ferrous ammonium sulfate with $K_2Cr_2O_7$)
10. Determination of composition of cuprammonium cation
11. Determination of strength of strong acid using pH meter.
12. Determination of strength of weak acid using pH meter.

Text Books:

1. Practical physical , B. Viswanadham and P.S. Raghavan, Viva Books pvt. Ltd., New Delhi, 2005
2. Experiments in physical Chemistry, J. C. Ghosh, Bharati Bhavan publishers, 2nd Ed., 1968

M.Sc. CHEMISTRY (PHARMACEUTICAL CHEMISTRY)
II SEMESTER
SCY 702: ADVANCED INORGANIC CHEMISTRY

Hours per week	: 4	Semester End Examination	: 60 Marks
Credits	: 4	Continuous Evaluation	: 40 marks

UNIT-I

Bioinorganic Chemistry: Metal ions in Biology; Molecular mechanism of ion transport acrossmembranes- ionophores; Photosynthesis; Nitrogen fixation; Oxygen uptake proteins - hemoglobin and myoglobin; Electron transfer proteins - Cytochromes and Ferrodoxins; Inorganic medicinal compounds - superoxide dismutage mimics, vanadium based diabetic drugs and platinum containing anticancer agents.

UNIT-II

Organometallic Chemistry: Introduction, Nomenclature, the 18-electron rule. Metal carbonyls,structure and bonding, vibrational spectra of metal carbonyls for bonding and structural elucidation, important reactions of metal carbonyls; preparation, bonding, structure and important reactions of transition metal nitrosyl, dinitrogen and dioxygen complexes; tertiary phosphine as ligand; Metallocenes-ferrocene; Catalysis by organometallic compounds - hydrogenation, hydroformylation, and polymerization.

UNIT-III

Metal Clusters: Higher boranes, carboranes, metalloboranes and metallocarboranes. Metal compounds with metal-metal multiple bonds. Preparation, properties and structures of $Re_2Cl_8^{2-}$, $Mo_2Cl_8^{4-}$, $Re_2(RCOO)_4X_2$, $Cr_2Cl_9^{3-}$, $W_2Cl_9^{3-}$, Re_3Cl_9, $Re_3Cl_{12}^{3-}$, $Mo_6Cl_8^{4+}$, $Nb_6Cl_{12}^{2+}$.

UNIT-IV

Solid State and Structural Chemistry: Crystal structures - close packing, body centered andprimitive structures; Symmetry in crystals, Crystallographic point groups; Description of structures - AB structures (NaCl, CsCl, ZnS), AB_2 structures (Rutile, Fluorite), A_2B_3 structures (β-Al_2O_3), ABO_3 structures (perovskite) and AB_2O_4Spinels.

UNIT V

Chemistry of Nanomaterials: Classification–zero, one and two dimentional nanomaterials.Synthesis and biomedical applications of gold, silver and iron oxide nanoparticles, Introduction to fullerenes and carbon nanotubes (SWCNTs, MWCNTs). Synthesis, Properties and applications of CNTs.

Text Books

1. Bioinorganic Chemistry by L. Bertini, H.B. Gray, J.S. Valentine, Uni. Science Books, 1994.
2. Bioinorganic Chemistry: A short course by Rosette M. Roat-Malone, John-Wiley Sons. Inc., 2002.
3. Inorganic Chemistry: Principles of Structure and Reactivity by James E. Huheey, Okhil K. Medhi Ellen A. Keiter, Richard L. Keiter, 2006.
4. Inorganic Chemistry, Gary L. Miessler and D. A. Tarr, 3rd Edition 2004, Pearson-Prentice Hall.
5. Textbook of Nanoscience and Nanotechnology by B.S. Murthy, Universities Press, 2012
6. „Nanochemistry: A chemical approach to Nanomaterials", Ozin Geoffrey A. and Andre C. Arsenault, Royal Society of Chemistry Publication, 2005.

SCY 704: REACTION MECHANISM AND HETEROCYCLIC COMPOUNDS

Hours per week	: 4	Semester End Examination	: 60 Marks
Credits	: 4	Continuous Evaluation	: 40 marks

UNIT-I

Aliphatic and Aromatic Substitution Reactions: Nucleophilic - The S_N2, S_N1, S_Ni and SETmechanisms, neighbouring group participation, anchimeric assistance, classical and non classical carbocations, phenonium ions, norbornyl system, allylic, aliphatic, trigonal and vinylic carbon, factors effecting substitutions.

Electrophilic -SE^1, $SE^2$and SE^iMechanisms and related effects.

UNIT-II

Elimination Reactions: The E2, E1 and E1cB mechanisms and their orientation of the doublebond. Reactivity-effects of substrate structure, attacking base, leaving group and the medium. Stereochemistry of eliminations in acyclic and cyclic systems, orientation in eliminations – Saytzeff and Hoffman elimination, Regio and stereo selectivity reactions.

UNIT-III

Basic concepts of some organic reactions: Aldol, Stobbe, Cannizaro, Wittig, Grignard,Reformatsky Reactions. Openauer oxidation, Clemmensen reduction , Birch reductions, Michael addition, Mannich Reaction, Diels - Alder reaction, Ene-reaction, Bayer - Villiger Reaction, Wolf-Kishner reduction, Favorskii reaction, Chichibabin reaction. Vilsmeier, Robinson annulation.

UNIT-IV

Synthesis and Reactivity of the compounds with one heteroatom: Pyrrole, Furan, Thiophene,Pyridine, Quinoline, Isoquinoline, Indole, Benzofuran and Benzothiophene.

UNIT-V

Synthesis and Reactivity of the compounds with more than one heteroatom Pyrazole,Imidazole, Oxazole, Isoxazole, Thiazole, Isothiazole, Pyridazine, Pyrimidine ,Pyrazine and Purine.

Text books:

1. Organic Chemistry Vol. I (Sixth Edn.) and Vol. II (Fifth Ed.,) by IL Finar ELBS., 2002
2. Organic Chemistry (fifth Edn.,) by Morrison and Boyd, PHI, India., 2011
3. Reaction Mechanism in Organic Chemistry by Mukherjee Singh, Macmillan, India., 2012
4. Heterocyclic compounds by Raj K Bansal ,New age International, 1999
5. Reaction Mechanism & reagent in Organic Chemistry,G.R.Chatwal,Himalaya Publishing House,2012.

Reference Books:

1. Advanced Organic Chemistry by Jerry March (3rd Edn.) Wiley Eastern., 2006
2. Organic Chemistry (fifth edition)by Francis A. Carey Tata Mac Graw Hill publishing company Limited, New Delhi, 2007

SCY 706: ELECTROCHEMISTRY AND SURFACE CHEMISTRY

Hours per week	: 4	Semester End Examination	: 60 Marks
Credits	: 4	Continuous Evaluation	: 40 marks

ELECTROCHEMISTRY

UNIT-I

Electrochemical cells: Measurement of EMF-Nernst equation-effect of complexation onelectrode potential; Polarization-Decomposition potential and overvoltage- Factors affecting overvoltage- Importance of over-voltage; Activity and activity coefficients- determination of mean ionic activity coefficient by EMF method; Debye-Huckel limiting law (DHLL) and its verification, Extended Debye-Huckel law; Debye-Huckel-Onsagar equation(derivation not required)-verification and its limitations

UNIT-II

Applications: Batteries-primary and secondary cells–lechlanche cell, lead acid storage battery,Nickel-Cadmium cell; Fuel cells-Oxygen-hydrogen fuel cell; Corrosion- theories of dry and wet corrosion-different forms of corrosion- prevention and control of corrosion - cathodic protection-sacrificial anodic and impressed current methods- inhibitors-anodic and cathodic inhibitors; protective coatings-galvanising and tinning

SURFACE CHEMISTRY

UNIT-III Adsorption

Gibbs adsorption isotherm, types of adsorption isotherms, solid-liquid interfaces, solid-gas interface, physisorption and chemisorption, , Langmuir and Freundlich isotherms. BET equation (derivation not required) and surface area determination. Kinetics of surface reactions involving adsorbed species, Langmuir-Hinshelwood mechanism

UNIT-IV Micelles

Surface active agents- classification- critical micellar concentration (CMC)- factors affecting the CMC of surfactants- determination of cmc, Solubilisation-factors influencing the solubilisation. Micellization-thermodynamics of micellization. Micro emulsions- comparision of microemulsions with conventional emulsions-applications. Reverse micelles.

UNIT-V Polymer chemistry

Basic concepts- monomers, repeat units, degree of polymerization, linear, branched and network polymers, classification of polymers. Polymerization-Free radical, ionic and co-ordination polymerization. Kinetics of condensation (step-growth), free-radical and ionic polymerizations. Physical characterization: Number and mass average molecular weights (Mn, Mw), Determination of molecular masses – Osmometry, viscometry and light scattering methods

Text Books:

1. Physical Chemistry – P. W. Atkins, Oxford University press, VIIth edition, 2002.
2. Electrochemistry for chemists- S. Glasstone, D. Van Nostrand , 1965
3. Physical Chemistry of macromolecules- D. D. Deshpande, Vishal Publications.
4. Micellar Catalysis (Surfactant Science series,vol.133)Mohammad Niyaz Khan.Taylor & Francis,2007
5. Micelles, Theoretical and applied aspects., V. Moroi, Plenum press, New York, 1992
6. A text book of Physical Chemistry Vol. 2,3 and 5 K.L.Kapoor, Macmillan, India Limited, 2004

SCY 708: QUANTUM CHEMISTRY AND GROUP THEORY

Hours per week	: 4	Semester End Examination	: 60 Marks
Credits	: 4	Continuous Evaluation	: 40 marks

Quantum Chemistry

UNIT-I

Wave equation-interpretation of wave function-properties of wave function-normalization and orthogonalisation, operators-linear and non linear commutators of operators. Postulates of quantum mechanics, setting up of operators observables- Hermitian operator-Eigen values of Hermitian operator Particle in one dimensional box.

UNIT-II

Particle in a three dimensional box, rigid rotor, wave mechanics of systems with variable potential energy- simple harmonic oscillator- solution of wave equation-selection rules.

UNIT-III

Approximation methods: Perturbation theory- application to ground state energy of Heliumatom; Variation principle-applications- calculation of zero point energy of harmonic oscillator. Many electron atom-Hartee-Fock Self consistent field method (qualitative treatment only).

UNIT-IV

Bonding in molecules: Born-Oppenheimer approximation- Hydrogen molecule ion, LCAO-MOand VB treatments of the hydrogen molecule (fundamental concepts only); electron density, forces and their role in chemical bonding. Hybridization and valence MOs of H_2O, NH_3 and CH_4. Huckel pi-electron theory and its applications to Ethylene, Butadiene and Benzene.

UNIT-V

Symmetry and Group Theory in Chemistry: Symmetry elements and symmetry operationsand point groups, Schoenflles symbols, classification of molecules into point groups, Axioms of group theory, group multiplication tables for C_{2v} and C_{3v} point groups, representations-reducible and irreducible representations, Mulliken symbols, orthogonality theorem (without proof) and its implications, Character table and its anatomy.

Text Books:

1. Introduction to Quantum Chemistry, A.K. Chandra, Tata McGraw Hill, 4th Ed.,(1994)
2. I.N. Levine, Quantum Chemistry, 5th Ed., (2000), Pearson Educ. Inc., New Delhi.
3. D.A. Mc Quarrie and J.D. Simon, Physical Chemistry: A Molecular Approach, (1998) Viva Books, New Delhi.
4. Symmetry and Spectroscopy of Molecules, K.Veera Reddy, New Age, 1988

SCY722: INORGANIC CHEMISTRY LAB

Hours per week	: 9	Semester End Examination	: 60 Marks
Credits	: 3	Continuous Evaluation	: 40 marks

1. **Inorganic Synthesis**
   Preparation of following complexes
   a) Tetraaminecopper(II) sulphate
   b) Potassium tris(oxalato) ferrate(III) trihydrate
   c) Potassium tris(oxalato) aluminate(III)
   d) Tris(thiourea) copper(I) sulphate
   e) Hexaaminecobalt(III) chloride

2. **Determination of metal ions**
   a) Zinc using potassium ferrocyanide
   b) Zinc using EDTA
   c) Magnesium using EDTA
   d) Cerium (IV) using potassium ferrocyanide
   e) Iron(III) by photochemical reduction method

3. **Separation of ions using Ion Exchange Chromatography**
   a) Zinc and Magnesium
   b) Chloride and Bromide

Books:

1 Vogel's Qualitative Inorganic Analysis - VIIth Edition Revised by G. Svehla, Pearson Education Ltd., 1996

SCY724: COMPUTATIONAL CHEMISTRY LAB

Hours per week	: 6	Semester End Examination	: 60 Marks
Credits	: 3	Continuous Evaluation	: 40 marks

CHEMDRAW:

Drawing the structure of simple aliphatic, aromatic, heterocyclic compounds with different substituent. Identification of IUPAC name

Operation of one or more packages such as EXCEL, MS Word and Power point

MATLAB:

Statistical Data Processing and Curve Fitting
Mean, Standard deviation, coefficient of variation of univariate data,
Determination of First order rate constant
Adherence to Beers law
Correlation coefficient
Quadratic and cubic curve fitting

CQC Studies:

Z-matrix
Geometry optimization by PM3, HF, B3LYP
Single point energy of water
Single point energy of formaldehyde
Geometry optimization of few molecules – water, methane, benzene, carbon tetrachloride and meta-dintrobenzene
Geometry optimization and MO energy of ethylene and butadiene
Frequency Analysis, stable compound, Transition state
Dipole moments, polarizabilites
Ionization potential, electron affinities
HOMO, LUMO, energies
ESP, Total electron density
Spectra: UV-Vis, infra red spectra

Text Books:

1. J. Foresman and A. Frisch, Exploring Chemistry with Electronic Structure Methods, Gaussian Inc., 2000.
2. Hehre W. J., Shusterman A. J. and Huang W. W., „A Laboratory Book of Computational Organic Chemistry", 1996.
3. Computer Fundamentals – Pradeep K. Sinha – BPB Publications – Fourth Edition
4. Working with Microsoft Office – by Ron Mansfield (Tata McGraw-Hill)
5. G.Grant and W. Richards, Computational Chemistry, Oxford University press.
6. Computer manuals:PC-MATLAB, the Mathworks, Inc., 1989

III SEMESTER

M.Sc. CHEMISTRY (PHARMACEUTICAL CHEMISTRY)
SOC 801: ORGANIC SYNTHESIS

Hours per week	: 4	Semester End Examination	: 60 Marks
Credits	: 4	Continuous Evaluation	: 40 marks

UNIT-I

Formation of carbon-carbon single bonds: Alkylations via enolate, enamine and relatedreactions, umplong (dipole inversion), carbon-carbon bond formation through organo lithium, organo palladium Heck reaction & Suzuki coupling. Organonickel and organocopper reagents. Thiocarbanions, selenocarbanions and sulphur ylides.

UNIT-II

Formation of carbon-carbon double bonds: Elimination reactions - pyrolytic, syn eliminations,sulphoxide-sulphinate rearrangement, Peterson reaction, Wittig reaction, alkenes form arylsluphonyl-hydrazones, Eschenmoser fragmentation, olefin metathesis (Grubbs reaction).

UNIT-III

Organoboranes: Preparation of Organoboranes, hydroboration, disiamyl borane, thexyl borane,9-BBN and diisocamphenyl borane, functional group transformations of organoboranes-oxidation, protonolysis and rearrangements. Formation, of carbon - carbon-bonds viz organoboranes, carbonylation, the cyanoboration process and reaction of alkenyl boranes.

Organosilanes: Synthetic applications of trimethylsilyl chloride, dimethyl-t-butylsilyl chloride,trimethylsilyl cyanide, synthetic applications of- α silyl carbanion and β-silyl carbonium ions.

UNIT-IV

Reduction: Catalytic hydrogenation (homogeneous and heterogeneous), reduction by dissolvingmetals, reduction by hydride transfer reagents, complex metal hydrides, reduction with hydrazine and diamide,

Oxidation: Oxidations of hydrocarbons, alkenes, alcohols aldehydes and ketones oxidativecoupling reactions. Use of Pb $(OAC)_4$, NBS, CrO_3, SeO_2, MnO_2, , $KMnO_4$, OsO_4. Wood ward and Provost hydroxylation.

UNIT – V

Retrosynthesis the disconnection approach: Introduction, terminology, principles convergentand linear synthesis, One group C–X (X = hetero atom),

C-C disconnections and two groups C–X and C-C disconnections with reference to 1,1; 1,2; 1,3; 1,4 and 1,5 difunctionalised compounds. Reterosynthesis and synthetic strategies with examples - salbutamol, benzocaine, paracetamol and dinocap.

Textbooks:

1. Some Modern Methods of Organic Synthesis W. Carruthers, Third Edition, Cambridge University, Press, Cambridge, 1988.
2. Organic Synthesis: The disconnection approach, S. Warran, John Wiley & sons, New York, 1984
3. Principles of Organic Synthesis by R.O.C. Norman, J.M.Coxon, N. Thernes, Black Academic & Professional, 1995
4. Advanced Organic Chemistry by Jerry March 3rd Ed., Wiley Eastern, 2010

Reference Books:

1. Organic Synthesis viz Boranes, Herbet C. Brown Gray, W. Kramer Alan B. Levy and M. Mark Midland John Wiely & Sons, New York, 1975.
2. Organic Chemistry By Carry Sandburg. Volume1 & II Springer., 2007

SPC 803: PHARMACEUTICAL CHEMISTRY

Hours per week	: 4	Semester End Examination	: 60 Marks
Credits	: 4	Continuous Evaluation	: 40 marks

UNIT-I

MOLECULAR BASIS OF DRUG ACTION

A) Receptor: Drug Receptor Interaction.
   a) Basic ligand concept, agonist, antagonist, partial agonist, inverse agonist.
   b) Receptor Theories - Occupancy, Rate & Activation Theories.
   c) Receptor Binding Assays, Determination of B-max and Kd by transforming data with Hill plot and Scatchered plot.

B) Drug binding to nucleic acid -- Antimalarial, anti-cancer, antiviral

UNIT-II

DESIGN AND APPLICATION OF PRODRUGS

a) Prodrug concept.
b) Prodrugs of various functional groups like carbonyl, hydroxy. amide, amines.
c) Application of Prodrug approach to:
   i. Improvement of bioavailability
   ii. Prevent first pass metabolism
   iii. Reduction of side effects
   iv. Prolong duration of action
   v. Site specific delivery

UNIT -III

ADMET Studies in Drug Discovery and Development

Physicochemical properties in relation to drug action; Introduction of ADMET; QSPR studies Importance of metabolic property of Drug; Metabolic transformation of drugs and its role in development of new drug molecules; Metabolic antagonism.

UNIT-IV

Stereochemical aspects of drug receptor interactions

(i) Stereochemical importance in mechanism of drug interaction with receptor.
(ii) Isosterism and bioisosterism as guides to structural variations
(iii) Concepts of conformational analysis and its role in design and development of new drug molecules.

UNIT-V

Chiral Technology:

Introduction to Chirality and Techniques used asymmetric synthesis of

Diltiazem, Vitamin C, Ampicillin, Dextrapropoxyphen, Propranolol.

Recommended Books

1. Burger: Medicinal Chemistry (John Wiley & Sons N.Y.)
2. Foe: Principles of Medicinal Chemistry (Varghese & Co.)
3. Ledinicer: Organic Drug synthesis (John Wiley & Sons N.Y.)

SPC 805: ANALYTICAL METHODS AND SPECTROSCOPY

Hours per week	: 4	Semester End Examination	: 60 Marks
Credits	: 4	Continuous Evaluation	: 40 marks

UNIT-I

Aqueous Chemistry: concepts and general applications in the analysis of pharmaceuticalsubstances: Neutralization Titrations: principle, titration curves and theory of acid base Indicators.

Complexation Titrations: Types of EDTA titrations, masking and de-masking agents. metalion indicators. **Precipitation Titrations**: principle, indicators for precipitation titrations Volhard method, Fajans method and Mohr‟s method.

Redox Titrations: Principle, redox indicators, Permagnatometry, and Dichromatometry, Iodometry & Iodimetry.

UNIT-II

Non- Aqueous Chemistry: concepts and general applications in the analysis of pharmaceutical substances: Characteristic of Non-aqueous solvents, non-aqueous titrations-types of reactions, indicators and applications: i). Determination of acids, ii) Determination of bases, iii) Karl-Fischer reagent for the determination of moisture content in drugs

UNIT III

Fundamentals of chromatography: Classification of chromatographic separation, isotherms, Chromatographic separation parameters, Chromatographuic media, methods of development in chromatography: Displace ment, Isocratic and gradient elution, Kinetic factors affecting chromatographic separation: Van Deemter equation, HETP and Resolution.

Planar chromatography: Thin layer chromatography: Principle, chromatographic media-coating materials, activation of adsorbent, development of chromatographic plate and visualization methods, applications. HPTLC - Principle and technique

Unit IV

High performance liquid chromatography: Basic principle and instrumentation: pumps, columns and detectors. Modes of HPLC: principle and general applications in assay of pharmaceutical substances: Capillary electrophoresis, affinity chromatography and Ion chromatography.

Gas liquid chromatography: principle, columns , detector. Concept of programmedtemperature Gas chromatography. General application in analysis of residual solvents.

Unit V

Basic principle , instrumentation and general applications of the following: UV-Visiblespectroscopy, Spectro-fluroscence spectroscopy, Infrared spectroscopy and Mass spectroscopy.

Books:

1. Principles and practice of Analytical Chemistry-F.W.Fifield and D.Kealey,Blackwell Science,2004

2. Separation Chemistry- R.P.Buddhiraja, New age international (P) Ltd.,Publishers,2004
3. Quantitative Analysis, R.A.Day & A.L.Underwood, Prentice -Hall of India,1991
4. Chemical analysis - H.A. Laitinan, McGraw Hill Book Co.,1975
5. D.A. Skoog, D.M. West and F.J. Holler, Analytical Chemistry, An Introduction, Sanders College Publishing, New York,2004
6. Analytical Chemistry Gary D Christian, John Wiley and Sons inc,2003.
7. Volumetric Analysis, Vol. III -I. M. Kolthoff and R. Welcher, Interscience Public, New York,1969
8. Vogel's textbook of Inorganic Quantitative Analysis - J. Bassett et al. ELBS ,2005

Reference Books:

1. Chromatography concepts and contrasts – J.M.Miller, Wiley Interscience,2005
2. R.P.W. Scott, Techniques and practice of Chromatography, Marel Dekker Inc., New York,1969.

SPC 841: QUALITY ASSURANCE AND REGULATORY AFFAIRS

Hours per week	: 4	Semester End Examination	: 60 Marks
Credits	: 4	Continuous Evaluation	: 40 marks

UNIT- I

Characteristics of an analysis: Classification of errors, accuracy-absolute and comparativemethod, propagation of errors, precision, significant figures, mean and standard deviation, the confidence limit, Test of significance-Q-test, T-test and F-test, control charts

UNIT- II

Quality assurance and management systems: Elements of quality, quality control, quality assurance, Triple role concept, quality process model. Customer requirement of quality, quality assurance in design, development, Statistical process control, statistical quality control and acceptance sampling

UNIT-III

Quality and quality management system: Quality objectives-ISO standards concept: ISO9000,ISO14000 and its requirements.

Good laboratory practice (GLP) – Introduction, history of GLP, Principles of good manufacturing practice, basic issues of GLP, GLP status in India

UNIT-IV

Calibration and maintenance of Equipment: Instrument calibration–linear calibrationcurves, , calibration of common laboratory instrument and equipment (Analytical balances, volumetric glassware, ovens, furnaces, UV / Visible spectrophotometer, pH meter, conductivity meter, IR).

Validation of analytical method- methodology, limit of detection, limit of quantification, range,sensitivity, selectivity and specificity, quality control-principles of Ruggedness/Robustness. .

UNIT-V

General idea regarding pharmaceutical industry.- Introduction, Definition and classificationof drugs, Quality of drugs, Sources of impurities in pharmaceutical chemicals and raw materials. Impurity profiling, classification of impurities, dissolution techniques of drugs, Significance of stability studies, types of stability studies, quantification of impurities. Basic concept of ICH guidelines for impurity profiling and stability studies.

Textbooks:

1. Quality Assurance and Quality Management in Pharmaceutical Industry, Y. Anjaneyulu, R.Marayya, Pharma Book syndicate, 2002.
2 Analytical Chemistry, Gary D Christian, John Wiley and Sons Inc, 2003.

Reference Books:

1. Fundamentals of Analytical Chemistry, An Introduction, D.A. Skoog, D.M. West F.J. Holler and S R. Crouch, Sanders College Publishing, New York, 2004
2. K.V.S.G. Murali Krishna, An introduction ISO 9000, ISO 1400 Series, Environmental Management
3. Analytical Method Development and Validation, Michael Swartz & Swartz Swartz, CRC press.1997
4. Quality Assurance in Analytical Chemistry, Wenclawiak, M.Koch, Spinger, Germany, 2006.

SPC 843: DRUG DESIGN AND DISCOVERY

Hours per week	: 4	Semester End Examination	: 60 Marks
Credits	: 4	Continuous Evaluation	: 40 marks

UNIT-I
Basic Principles of Drug Design

Introduction, Drug Design, conceptual, practical and humanitarian approaches; definition, and properties of drug molecule, physiochemical properties, shape, stereochemical and electronic properties of drug molecule

UNIT-II
Non Messenger targets for Drug action
Acetylcholine and Cholinergic receptors, Norepinephrine and Adrenergic receptors, Dopamine and Dopaminergic receptors, Serotonin and Serotonergic receptors, Histamine and Histamine receptors

UNIT-III
Targets for Drug Action
Drug design targeting viruses, bacteria, fungi and parasites. Drug design for therapies and antidotes for toxins. The clinical – molecular interface: Pneumonia, Meningitis and Encephalitis.

UNIT-IV
Enzymes in Drug design
Enzyme design using steroid template, Enzymes in synthetic organic chemistry, Enzyme- analog-Built polymers, Remote fictionalization reactions, Host- Guest complexation chemistry, Antibodies as enzymes,

UNIT-V
Pathways for drug deactivation and elimination
Oxidative reactions: aromatic hydroxylation, alkene epoxidation, oxidation of carbon nitrogen systems, Reduction reactions: Carbonyl reductions, nitro reductions, azo reduction

Carboxylation reactions, hydrolytic reactions; Conjugation reactions: Glucuronic acid conjugation, Sulphate conjugation, amino acid conjugation and acetyl conjugation.

Text books:

1. Bioorganic Chemistry Models and Applications. F.P.Schmidtchen. Springer
2. Medicinal Chemistry A Molecular and Biochemical approach Thomas Nogrady, Donald F. Weaver. Oxford University Press
3. Medicinal Chemistry revised edition, Rama Rao Nadendla. Pharma Med Press.
4. Bioorganic Chmeistry A Chemical approach to Enzyme Action Third edition Hermann Dugas, Springer.

Reference books:

1. The Organic Chemistry of Drug Design and Drug Action second edition Richard B. Silverman. Elsevier academic press.
2. Essentials of Medicinal Chemistry, second edition. Andrejus Korolkovas. Wiley India edition

SPC 845: INDUSTRIAL HYGIENE AND SAFETY

Hours per week	: 4	Semester End Examination	: 60 Marks
Credits	: 4	Continuous Evaluation	: 40 marks

UNIT-I

Introduction to Industrial Hygiene & Historical views, Definitions and professionals involved in industrial Hygiene work.

UNIT-II

Industrial safety aspects related to toxicity, noise, pressure, temperature, vibrations, radiations, etc. Explosions due to different forms of materials such as dust, vapour cloud, mist etc.

UNIT-III

Safety and Hygiene aspects related to

i. Transport, handling & storage of inflammable liquids & gases & toxic materials

ii. Process equipment including piping (fire, static electricity, pressure, temperature etc.) safety aspects at process development & design stage. Reliability engineering. Hazard mitigation systems, Emergency planning. Case studies.

UNIT-IV

Threshold Limit Value (TLV) and Permissible Exposure Limits (PEL) for chemicals, Industrial toxicology and the basics, Classification of toxic agents.

UNIT-V

Hazard identification, assessment & safety audit, HAZOP, HAZAN & consequence analysis.

Text Books:

1. Heinrich H.W. “Industrial Accident Prevention” McGraw-Hill Company, New York, 1980.
2. Krishnan N.V. “Safety Management in Industry” Jaico Publishing House, Bombay,1997.
3. Lees, F.P., “Loss Prevention in Process Industries” Butterworth publications, London, 2nd edition, 1990.
4. John Ridley, “Safety at Work”, Butterworth and Co., London, 1983.
5. Lees, F.P. “Loss Prevention in Process Industries” Butterworths and Company, 1996.

References:

1. “Quantitative Risk Assessment in Chemical Process Industries” American Institute of Chemical Industries, Centre for Chemical Process safety.
2. 2. Fawcett, H.h. and Wood, “Safety and Accident Prevention in Chemical Operations” Wiley inters, Second Edition.
3. “Accident Prevention Manual for Industrial Operations” NSC, Chicago, 1982.
4. GREEN, A.E., “High Risk Safety Technology”, John Wiley and Sons,. 1984.
5. Petroleum Act and Rules, Government of India.
6. Carbide of Calcium Rules, Government of India.

SPC 821: ORGANIC SYNTHESIS LAB

Hours per week	: 9	Semester End Examination	: 60 Marks
Credits	: 3	Continuous Evaluation	: 40 marks

Multistage organic synthesis:

Synthesis and purification of about six organic compounds involving three or more stages.

SPC823: ANALYTICAL METHODS AND SPECTROSCOPY LAB

Hours per week	: 6	Semester End Examination	: 60 Marks
Credits	: 3	Continuous Evaluation	: 40 marks

1. Limit tests :

a) Insoluble Matter by quantitative analysis
b) Chlorides, Sulphate, Nitrate and Oxalate
c) nonmetallic impurities: Boron ans Selenium

2. Aqueous Acid Base Titrations

a)Determination of sodium salicylate
b)Determination of Zinc oxide
c) Determination of Benzoic acid and Lactic acid

3) Non Aqueous Acid Base Titrations : Titration of Primary amines with perchloric acid

4. Redox Titrations:

a)Titration of sodium nitrite by permagnatometry
b) Titration of ferrous fumarate with ceric ammonium sulphate
c) Idodimetric titration of Analgin
d) Iodometric titration of ferric ammonium citrate
e) Titration of sodium salicylate with potassium bromated

5. Precipitation titration: Titration of amide by argentometry

6. Complexometric Titration: Titration of alum

7. Spectrophotometry:

b)Determination of Nitrite
c)Determination of Phosphate

Demo:

Determination of moisture content in pharmaceutical samples by Karl Fisher method
Determination of Riboflavin by Spectrofluorimetry Infrared spectroscopy for quantitative analysis

IV SEMESTER

M.Sc. CHEMISTRY (PHARMACEUTICAL CHEMISTRY)

SOC 844: MEDICINAL CHEMISTRY

Hours per week	: 4	Semester End Examination	: 60 Marks
Credits	: 4	Continuous Evaluation	: 40 marks

UNIT-I

Drug discovery and design: Lead discovery and lead modification, structure modification toincrease bioavailability, lipophilicity, relationship between chemical structure and biological activity (SAR), QSAR- basic Concepts. Basic reactions of drug molecule synthesis.

UNIT-II

Drug structure and biological activity: Pharmaceutically important functional groups- alcohols, carboxylic acid, amines, sulfonamides and carbonyl compounds.
Chemistry of drug metabolism- absorption distribution, drug metabolism and excretion site specificity, stability, prolong release, minimum toxicity, patient acceptance.

UNIT-III

Vitamines : Structure, physiological role and uses of Vitamins A ,Vitamin DThiamine (B1) and Pyridoxine (B6).
Chemistry of selected drugs- Synthesis and basic concept of action for the following drugs

UNIT-IV

(i) Anticancer: 5-Fluorouracil, Vincristine
(ii) Antimalarial**s :**Chloroquine , Chloroguanide
(iii) Anti-inflammatory**:** Ibuprofen, Diclofenac Sodium
(iv)Sedatives: Phenobarbital, Lidocaina.

UNIT-V

(i) Antiulcers and antacids: Omeprazole, Ranitidine
(ii) Antiviral: Acyclovir
(iii) Antihistaminic: Terfenadine, Cinnarizine
(iv) Antiasthmatic agents : Salbutamol and Beclomethasone Dipropionate

Books Recommended

1. A. Burger, Medicinal Chemistry, Vol. I-III, Wiley Interscience Publications, New York (1995).
2. W. O. Foye, Principles of Medicinal Chemistry, 3rd Edition (1989), Lea & Febiger/ Varghese Publishing House, Bombay.
3. A. Kar, Medicinal Chemistry, Wiley Eastern Ltd., New Delhi (1993).
4. 4. Richard B. Silverman; The Organic Chemistry of Drug design and Drug action,II Ed.;
5. Rama Rao Nadendla;Medicinal Chemistry;PharmaMed Press, 2013
6. Glenn L.Jenkins,Walter H.Hartung,Kenneth E.Hamlin Jr.,John B.Data;The Chemistry of Organic Medicinal Products;IV Ed.; PharmaMed Press, 2010

Reference book

1. Andrejus Korolkovas ; Essentials of Medicinal Chemistry,II Ed. ,Wiely India, 2008
2. Thomas Nogrady,Donald F.Weaver; Medicinal Chemistry: A molecular and Biochemical approach; III Ed.:Oxford University Press , 2007

SPC 842: ADVANCED INSTRUMENTATION TECHNIQUES

Hours per week	: 4	Semester End Examination	: 60 Marks
Credits	: 4	Continuous Evaluation	: 40 marks

UNIT I

Flame photometry: Theory and instrumentation. Analyses of Na, K, Ca, and Mg.
Atomic Absorption Spectrometer: Theory, instrumentation, chemical and spectralinterferences, Applications

Induced couple plasma spectroscopy: Theory, Instrumentation and applications of ICP-OES

UNIT II - X-ray Spectroscopy: X-ray spectrometers, energy dispersive and wavelengthdispersive techniques, instrumentation, matrix effects and applications.

UNIT-III-Voltametry: Principle of polarography residual current, migration current, diffusioncurrent, half-wave potential, Ilkovic equation. Instrumentation: Dropping mercury electrode (DME), advantages and disadvantages of DME, qualitative and quantitative analysis of inorganic ions - Cu, Pb Cd and Zn. Anode Stripping Voltametry: Principle and instrumentation. Hanging drop mercury electrode, application in the analysis of some selected metals

UNIT IV- Thermal methods of analysis: Thermo gravimetry- theory, instrumentation,applications with special reference to $CuSO_4$. $5H_2O$, $CaC_2O_4.H_2O$ and $CaCO_3$. Basic idea of differential thermal analysis: principle and instrumentation. Difference between TGA and DTA. Differential scanning calorimetry: principle and instrumentation.

UNIT V

Capillary Electrophoresis: Principle, Factors Affecting Ionic Migration. Effect of Temperature. pHand Ionic Strength. Electro- osmosis supporting medium. Instrumentation, Modes : polyacrylamide gel electrophoresis, capillary zone electrophoresis, micellar electrokinetic electrophoresis, capillary gel electrophoresis and Isoelectric focusing and applications of capillary electrophoresis.

Elementary Idea of Hyphenated Techniques: Theory, interfaces in hyphenation of thetechnique and applications of the following:

LC –MS, GC –MS, CE-MS

Textbooks:

1. Instrumental methods of analysis - H.H. Willard, Meritt Jr. and J.A. Dean,CBS Publishers and distributors, 6th edition, 1986.
2. Principles of instrumental analysis – Douglas A. Skoog, F. James Holler and R. Crouch, Cengage Learning, 6th edition, 2006.
3. Vogel‟s textbook of Quantitative Inorganic analysis - J. Basset, R.C. Denney, G.H. Jeffery and J. Mendham, Prentice Hall, 6th edition, 2000
4. Industrial methods of analysis - B.K.Sarma, Goel Publishing House, Meerut, 1997
5. Instrumental methods of Analysis – G.R. Chatwal and S. Anand, Himalaya publishing House, 13th reprint, 1999.
6. Analytical Chemistry – S.Usha Rani, Macmillan India Limited, 2001

Reference Books:

1. Instrumental methods of Analysis – Galen S. Ewing, Mcgraw Hill Higher Education, 5th edition, 1985
2. Handbook of Instrumental techniques for Analytical Chemistry, Frank Settle, Prentice Hall, 1997.

IV SEMESTER

M.Sc. CHEMISTRY (PHARMACEUTICAL CHEMISTRY)

SCY 842: GREEN CHEMISTRY

Hours per week	: 4	Semester End Examination	: 60 Marks
Credits	: 4	Continuous Evaluation	: 40 marks

UNIT- I:

Introduction to Green Chemistry

Green chemistry - Introduction - need for green chemistry - goals of green chemistry - Anastas' twelve principles of green chemistry - Designing a green synthesis (tools) - choice of starting materials, solvents, catalysts, reagents, processes with suitable examples.

UNIT -II

Ionic liquids - synthesis, physical properties of ionic liquids - applications in alkylation,epoxidation, Friedal-Crafts reaction - Diels-Alder reactions – Knoevengal condensations and Wittig reactions.

Phase Transfer Catalyst (PTC) - Definition - advantages, types of PTC reactions - synthesisof PTC, applications of PTC in organic synthesis - Michael reaction - alkylation of aldehydes and ketones. Wittig, generation of dihalocarbene, elimination reaction

UNIT -III

Supercritical CO_2- phase diagram - uses in extracting natural products, dry cleaning,bromination, Kolbe-Schmidt synthesis - Friedel-crafts reaction. Dimethyl carbonate as a methylating agent in green synthesis

UNIT -IV

Microwave and Ultrasound Assisted Reactions

Microwave activation - advantages of microwave exposure - Microwave assisted reactions, condensation reactions - oxidation, reduction reactions, multicomponent reactions.

Sonochemistry - use of ultrasound in organic synthesis (alternate source of energy) - saponification - substitution, addition, oxidation reactions, reductions.

UNIT-V

Green Analytical Techniques

Micelle mediated extraction- Cloud point extraction and adsorptive miceller flocculation methods. Solid Phase Micro Extraction (SPME)

Text books:

1. Paul T. Anastas and John C. Warner, “Green Chemistry”, Oxford University Press,Indian Edition, 2008.
2. V. K. Ahluwalia and M. Kidwai, “New Trends in Chemistry”, Anamaya Publishers, 2nd Ed., 2007.
3. V. Kumar, “An Introduction to Green Chemistry”, Vishal Publishers, 1st Edition, 2007.
4. V. K. Ahluwalia and R. S. Varma, “Green Solvents”, Narosa Publishing, 1st Edition, 2009.
5. V.K.Ahluwalia and Renu Aggarwal, “Organic Synthetic Special Techniques”, Narosa,
6. V. K. Ahluwalia, “Green Chemistry - Environmentally Benign Reactions”, Ane books, India, 2006.

SOC802: CHEMISTRY OF NATURAL PRODUCTS

Hours per week	: 4	Semester End Examination	: 60 Marks
Credits	: 4	Continuous Evaluation	: 40 marks

Study of isolation, structural elucidation, stereochemistry, synthesis, biosynthesis of the following biological active classes of natural products.

UNIT-I
Microbial metabolites and shikimates : Pencillin G, Cephalosphorin-C, Prostaglandin 15 (R) PGA_2 Podophylotoxin and Etoposide.

UNIT-II
Terpenoids: Forskolin, Taxol, Azadirachtin, and Santonin

UNIT - III
Steroids: Cholesterol, Progesterone, Testosterone and Esterone

UNIT -IV
Alkaloids: Morphine, Reserpine, Camptothecin and Strychnine

UNIT -V
Nucleic acids: Basic concepts of the structures of RNA and DNA and their hydrolysis products: nucleotides, nucleosides and heterocyclic bases.

Text Books:

1. Organic Chemistry, Volume 2, Stereochemistry and chemistry of Natural products, I.L. Finar, 5th Edition, ELBS, 2002
2. Chemical Aspects of Biosynthesis, John Mann, Oxford University Press, Oxford, 1996
3. Chemistry of Natural Products: A Unified Approach, N.R. Krishnaswamy, University Press (India) Ltd., Orient Longman Limited, Hyderabad, 1999.
4. Introduction to Organic Chemistry, A Streitweiser, CH Heathcock and E.M/ Kosover IV Eeition, Mc.Milan, 1992.

SPC822: SPECTROSCOPY AND CHROMATOGRPY LAB

Hours per week	: 9	Semester End Examination	: 60 Marks
Credits	: 3	Continuous Evaluation	: 40 marks

- Separation and purification of organic compounds by making use of Thin layer Chromatography and Column Chromatography.
- Identification of functional groups by using IR and UV spectrophotometer
- Interpretation of given NMR spectra and identification of organic Compounds

SPC824: INSTRUMENTAL METHODS OF ANALYSIS LAB

Hours per week: 6 | Semester End Examination: 60 Marks
Credits: 2 | Continuous Evaluation: 40 marks

1.pH metry:

a) Determination of Boric Acid

2.Conductometry:

a)Determination of Aspirin

b) Determination of Ascorbic acid

3.Potentiometry: Determination of mixture of Chloride, Bromide and Iodide with silver nitrate

4.Nephelometry : Limit test for Chlorides and Sulphate by Nephelo-turbidimetric method

5. Flame photometry : Determination of Sodium and Potassium in calcium acetate

6. Spectrophotometry:

a)Determination of Phenol

b)Determination of Fe^{2+}

c) Determination of aspirin

d)Determination of Nickel(II)

e)Determination of Chromium(VI)

7. Polarimetry : Determination of optical rotation of pharmaceutical substances

8. Refractometry

a)Determination of Refractive index of pharmaceutical substances

b) Determination of CMC with Refractometry

Demo:

1) Assay of pharmaceutical tablet dosage forms by Isocratic HPLC method

2) Determination of caffine by stripping voltametry

SPC 892: PROJECT WORK (Credits: 8)

Students are required to carry out a project in the fourth semester of their study, under the supervision of a faculty member of the department. The results are to be submitted in the form of a dissertation. Project work shall be evaluated by two examiners at the semester end examination

Note:

Open electives: A student may choose open electives from the list of courses offered by anyinstitute of GITAM University