

FACULTY OF APPLIED SCIENCES

SYLLABUS

FOR

M.Sc. CHEMISTRY

(SEMESTER: I-IV)

(Under Choice based Credit System)

Examinations: 2021 Onwards

For

**University Main Campus, Constituent Campuses
and Affiliated colleges**

I K GUJRAL PUNJAB TECHNICAL UNIVERSITY

Note:

(i) Subject to change in the syllabi at any time. Please visit the University website time to time.

IK Gujral Punjab Technical University

VISION

To be an institution of excellence in the domain of higher technical education that serves as the fountainhead for nurturing the future leaders of technology and techno- innovation responsible for the techno-economic, social, cultural and environmental prosperity of the people of the State of Punjab, the Nation and the World.

MISSION

To provide seamless education through the pioneering use of technology, in partnership with industry and society with a view to promote research, discovery and entrepreneurship and

To prepare its students to be responsible citizens of the world and the leaders of technology and techno-innovation of the 21st Century by developing in them the desirable knowledge, skill and attitudes base for the world of work and by instilling in them a culture for seamlessness in all facets of life.

OBJECTIVES

- To offer globally-relevant, industry-linked, research-focused, technology- enabled seamless education at the graduate, postgraduate and research levels in various areas of engineering & technology and applied sciences keeping in mind that the manpower so spawned is excellent in quality, is relevant to the global technological needs, is motivated to give its best and is committed to the growth of the Nation;
- To foster the creation of new and relevant technologies and to transfer them to industry for effective utilization;
- To participate in the planning and solving of engineering and managerial problems of relevance to global industry and to society at large by conducting basic and applied research in the areas of technologies. To develop and conduct continuing education programmes for practicing engineers and managers with a view to update their fundamental knowledge base and problem-solving capabilities in the various areas of core competence of the University;

- To develop strong collaborative and cooperative links with private and public sector industries and government user departments through various avenues such as undertaking of consultancy projects, conducting of collaborative applied research projects, manpower development programmes in cutting-edge areas of technology, etc;
- To develop comprehensive linkages with premier academic and research institutions within the country and abroad for mutual benefit;
- To provide leadership in laboratory planning and in the development of instructional resource material in the conventional as well as in the audio- visual, the video and computer-based modes;
- To develop programmes for faculty growth and development both for its own faculty as well as for the faculty of other engineering and technology institutions;
- To anticipate the global technological needs and to plan and prepare to cater to them;
- To interact and participate with the community/society at large with a view to inculcate in them a feel for scientific and technological thought and endeavour; and
- To actively participate in the technological development of the State of Punjab through the undertaking of community development programmes including training and education programmes catering to the needs of the unorganized sector as well as that of the economically and socially weaker sections of society.

ACADEMIC PHILOSOPHY

The philosophy of the education to be imparted at the University is to awaken the **“deepest potential”** of its students as holistic human beings by nurturing qualities of self-confidence, courage, integrity, maturity, versatility of mind as well as a capacity to face the challenges of tomorrow so as to enable them to serve humanity and its highest values in the best possible way.

Department of Chemical Sciences

VISION

The Chemical Sciences at IKGPTU campus will address the challenging and important questions in the physical and life sciences of current era using its multi-disciplinary vision, its culture of synergistic collaboration and translational science, and its excellence in the physical, medical and engineering sciences. Chemical Sciences Department continues to explore the new fields and frontiers and, with them, fundamentally new and innovative ways to address the increasingly complex scientific, health, energy and environmental problems of our time.

MISSION

- Inspiring and educating undergraduate students in chemistry and molecular-driven sciences in the core concepts of chemistry and the scientific methodology.
- To explore the new frontier area of organometallic catalysis in synthetic chemistry.
- Developing more-economic and greener strategies for chemical synthesis and production
- Understanding how molecules and materials behave, interact and transform at macroscopic, molecular, atomic and electronic levels, and exploring the contribution of geometric and electronic structure to function.
- Informing the public about the excitement of science, its impact on everyday life, and the crucial role it plays in human health, energy and environmental stewardship
- Building centralized, state-of-the-science facilities designed to promote collaborative synergies among faculty, staff and students and across disciplinary boundaries.
- Sharing the excitement of new chemical knowledge across IKGPTU and to other institutions, educators, and the global community through scientific communications and outreach.

TITLE OF THE PROGRAM: M.Sc. CHEMISTRY

YEAR OF IMPLIMENTATION: New Syllabus will be implemented from June 2018 onwards.

DURATION: The course shall be two years, with semester system (4 semesters, with two semesters in a year). The Choice based credit system will be applicable to all the semesters.

ELGIBILITY FOR ADMISSION: Candidates with 50% marks (5% relaxation for reserved categories) in Bachelors Degree with Chemistry as one of the subject are eligible for admission to this course.

INTAKE CAPACITY: 25 (Twenty five)

MEDIUM OF INSTRUCTION: English.

PROGRAM EDUCATIONAL OBJECTIVES:

The Program Educational Objectives are the knowledge skills and attitudes which the students will acquire during post-graduation.

| | |
|------|--|
| PEO1 | Apply the scientific knowledge of Physics, Mathematics and Chemistry specialization for deeper understanding of the nature. |
| PEO2 | Identify, formulate, research literature, and analyze advanced scientific problems reaching substantiated conclusions using first principles of mathematics, natural sciences, and engineering sciences. |
| PEO3 | Design solutions for advanced scientific problems and design system components or processes. |
| PEO4 | Use research-based knowledge and research methods including design of experiments, analysis and interpretation of data, and synthesis of the information to provide valid conclusions. |
| PEO5 | Create, select, and apply appropriate techniques, resources and modern scientific methods with an understanding of the limitations. |
| PEO6 | Apply reasoning using contextual knowledge to assess health, safety, legal and cultural issues of society. |
| PEO7 | Communicate effectively on research based activities with the scientific community and society at large so as to comprehend and write effective reports and design documentation. |
| PEO8 | Recognize the need for, and have the preparation and ability to engage in independent and life-long learning in the broadest context of scientific and technological change. |

PROGRAM OUTCOMES: At the end of the program, the student will be able to:

| | |
|-----|---|
| PO1 | Apply principles of various concepts in understanding, analysis and prediction of scientific problems. |
| PO2 | Development of problem solving skill, critical thinking and analytical reasoning as applied to scientific problems. |
| PO3 | To introduce advanced ideas and techniques required in emerging scientific areas. |
| PO4 | To develop human resource with specialization in science along with various experimental techniques required for career in academia and industry. |
| PO5 | Engage in lifelong learning and adapt to changing professional and societal needs. |
| PO6 | Communicate effectively scientific information both in written and oral formats. |

PROGRAM SPECIFIC OUTCOMES:

At the end of the program,

| | |
|------|--|
| PSO1 | Students will be competent to provide solutions for challenges related to energy, environment, materials and health/medicine. |
| PSO2 | Students will be skilled in problem solving, critical thinking and analytical reasoning as applied to problems related to chemical sciences. |
| PSO3 | The students will acquire in-depth knowledge to understand and critically interpret the chemical literature. |
| PSO4 | Students will be able to address social, economic, and environmental issues. |
| PSO5 | Students will be able to design and carry out scientific experiments and analyze the results of such experiments. |
| PSO6 | Students will be able to explore new areas of research in both chemistry and allied fields of science and technology. |
| PSO7 | Students will be able to integrate knowledge of mathematics, physics and other disciplines to solve social and technological issues. |

SCHEME OF THE PROGRAM:

| Semester-I | | | | | | | | |
|-------------------|--------------------------------|---|------------------------------------|-------|---------|--------------------|------------|------------|
| Sr. No | Code | Theory Papers | Hours | L-T-P | Credits | Marks Distribution | | Marks |
| | | | | | | Internal | External | |
| 1. | CHL401-18 | Inorganic Chemistry-I | 45 | 4-0-0 | 4 | 30 | 70 | 100 |
| 2. | CHL402-18 | Reactive Intermediates-I | 45 | 4-0-0 | 4 | 30 | 70 | 100 |
| 3. | CHL403-18 | Physical Chemistry-I | 45 | 4-0-0 | 4 | 30 | 70 | 100 |
| 4. | CHL404-18 | Spectroscopy - I | 45 | 4-0-0 | 4 | 30 | 70 | 100 |
| 5. | CHL405-18 | Environmental Chemistry | 45 | 3-0-0 | 3 | 25 | 50 | 75 |
| 6. | CHL406A-18 Or CHL406B-18 | Human Physiology * Or Numerical Methods for chemists* | 45 | 3-0-0 | 3 | 25 | 50 | 75 |
| 7. | CHP407-18 | Inorganic Chemistry Lab | 60 | 0-0-6 | 3 | 50 | 25 | 75 |
| 8. | CHP408-18 | Organic Synthesis Lab | 60 | 0-0-6 | 3 | 50 | 25 | 75 |
| | | Total | 28 (Theory 22, Practical 6) | | | 270 | 430 | 700 |

| Semester-II | | | | | | | | |
|--------------------|--------------------------------|--|------------------------------------|-------|---------|--------------------|------------|------------|
| Sr. No | Code | Theory Papers | Hours | L-T-P | Credits | Marks Distribution | | Marks |
| | | | | | | Internal | External | |
| 1. | CHL411-18 | Inorganic Chemistry-II | 45 | 4-0-0 | 4 | 30 | 70 | 100 |
| 2. | CHL412-18 | Reactive Intermediates-II | 45 | 4-0-0 | 4 | 30 | 70 | 100 |
| 3. | CHL413-18 | Physical Chemistry-II | 45 | 4-0-0 | 4 | 30 | 70 | 100 |
| 4. | CHL414-18 | Spectroscopy - II | 45 | 4-0-0 | 4 | 30 | 70 | 100 |
| 5. | CHL415A-18 Or CHL415B-18 | Chemistry of Materials Or Chemical Biology | 45 | 4-0-0 | 4 | 30 | 70 | 100 |
| 6. | CHP416-18 | Physical Chemistry Lab | 60 | 0-0-6 | 3 | 50 | 25 | 75 |
| 7. | CHP417-18 | Advanced Chemistry Lab-I | 60 | 0-0-6 | 3 | 50 | 25 | 75 |
| | | Total | 26 (Theory 20, Practical 6) | | | 250 | 400 | 650 |

| Semester-III | | | | | | | | |
|---------------------|--|---|------------------------------------|-------|---------|--------------------|------------|------------|
| Sr. No | Code | Theory Papers | Hours | L-T-P | Credits | Marks Distribution | | Marks |
| | | | | | | Internal | External | |
| 1. | CHL501-18 | Inorganic Chemistry-III | 45 | 4-0-0 | 4 | 30 | 70 | 100 |
| 2. | CHL502-18 | Advanced Organic Chemistry –I | 45 | 4-0-0 | 4 | 30 | 70 | 100 |
| 3. | CHL503-18 | Physical Chemistry-III | 45 | 4-0-0 | 4 | 30 | 70 | 100 |
| 4. | CHL504-18 | Advanced Characterization Techniques | 45 | 4-0-0 | 4 | 30 | 70 | 100 |
| 5. | CHL505A-18 Or CHL505B-18 Or CHL505C-18 | Biophysical chemistry Or Medicinal Chemistry Or Advanced Functional Materials | 45 | 4-0-0 | 4 | 30 | 70 | 100 |
| 6. | CHP506-18 | Advanced Chemistry Lab- II | 60 | 0-0-6 | 3 | 50 | 25 | 75 |
| 7. | CHP507-18 | Dissertation ** | | 0-0-8 | 4 | 50 | - | 50 |
| | | Total | 27 (Theory 20, Practical 7) | | | 250 | 375 | 625 |

| Semester-IV | | | | | | | | |
|--------------------|--|---|---|--------|---------|--------------------|------------|------------|
| Sr. No | Code | Theory Papers | Hours | L-T-P | Credits | Marks Distribution | | Marks |
| | | | | | | Internal | External | |
| 1. | CHL511-18 | Advanced Organic Chemistry- II | 45 | 4-0-0 | 4 | 30 | 70 | 100 |
| 2. | CHL512A-18 Or CHL512B-18 Or CHL512C-18 Or CHL512D-18 Or CHL512E-18 Or CHL512F-18 | Advanced physical Chemistry Or Chemical Toxicology Or Supramolecular Chemistry Or Chemistry of Natural Products Or Green Chemistry Or Computational Chemistry | 45 | 4-0-0 | 4 | 30 | 70 | 100 |
| 3. | CHP513-18 | Research Seminar | 30 | | 3 | 50 | - | 50 |
| 4. | CHP514-18 | Dissertation ** | | 0-0-24 | 12 | 150 | 100 | 250 |
| | | Total | 23 (Theory 8, Practical 12, Seminar 3) | | | 260 | 240 | 500 |

* Human Physiology for students with mathematical background and Numerical methods for chemists for students with medical background.

** Dissertation work will begin in third semester and will be continued in fourth semester. At the end of third semester, students will submit their literature work in the form of a review on the topic selected. There will be a presentation before a panel of teachers from the department.

EXAMINATION AND EVALUATION

| THEORY | | | | |
|-----------|--|--------------------|----|---|
| S.No. | | Weightage in Marks | | Remarks |
| 1 | Mid-Semester Examination | 20 | 15 | MSTs, Quizzes, assignments, attendance, etc. Constitute internal evaluation. Average of two mid-semester exams will be considered for evaluation |
| 2 | Attendance | 5 | 5 | |
| 3 | Assignments | 5 | 5 | |
| 4 | End-Semester Examination | 70 | 50 | Conduct and checking of the answer sheets will be at the department level in case of university teaching department of Autonomous institutions. For affiliated colleges examination will be conducted at the university level |
| | Total | 100 | 75 | |
| PRACTICAL | | | | |
| 1 | Daily evaluation of practical performance/ record/ viva voce | 30 | | Internal Evaluation |
| 2 | Attendance | 5 | | |
| 3 | Internal Practical Examination | 15 | | |
| 4 | Final Practical Examination | 25 | | External Evaluation |
| | Total | 75 | | |

PATTERN OF END-SEMESTER EXAMINATION

- I. **Part A** will be One Compulsory question consisting of short answer type questions [Q No. 1(a-j)] covering whole syllabus. There will be no choice in this question. It will be of 20 marks comprising of **10 questions of 2 marks each**.
- II. **Part B** will be comprising of eight questions [2-9]. Student will have to attempt any six questions from this part. It will be of 30 marks with **6 questions of 5 marks each**.
- III. **Part C** will be comprising of two compulsory questions with internal choice in both these questions [10-11]. It will be of 20 marks with **2 questions of 10 marks each**.

SYLLABUS OF THE PROGRAM

The syllabus has been upgraded as per provision of the UGC module and demand of the academic environment. The contents of the syllabus have been duly arranged unit wise and included in such a manner so that due importance is given to requisite intellectual and laboratory skills. The application part of the respective contents has been appropriately emphasized.

SEMESTER-I

| I.K. GUJRAL PUNJAB TECHNICAL UNIVERSITY DEPARTMENT OF CHEMICAL SCIENCES | |
|--|--|
| Course Name | M.Sc. Chemistry |
| Subject Code: | CHL401-18 |
| Subject Title: | INORGANIC CHEMISTRY-I |
| Contact Hours: | L:4 T:0 P:0 Credits:4 |
| Examination Duration (hours) | 3 |
| Objective(s): | The aim and objective of this course is to teach the fundamental and advanced concepts of chemistry of transition metals and their magnetic chemistry to the students. |

Details of the Course

| Unit | Contents | Contact Hours |
|-------------|---|----------------------|
| I | Coordination Chemistry: Coordination complexes, ligands and their classification, chelation and chelate effect, Werner's coordination theory, nomenclature, stability of complex and stability constants, stereochemistry, isomerism, Valence bond theory: postulates, examples of complexes, shortcomings. Crystal Field Theory d-orbital by electrostatic field (octahedral, tetrahedral and square planar geometry), and magnetic properties (high spin and low spin complexes); factors affecting crystal field splitting energy (10 Dq value), nephelauxetic effect and spectrochemical series; Structural and thermodynamic effects of d-orbital splitting (variation of ionic radii, Jahn-Teller effect, hydration and lattice energies of first row transition metal ions) | 12 |
| II | Transition Metals Chemistry I: LS coupling, derivation of spectroscopic terms for d ¹ to d ⁹ electronic configurations, correlation diagram for d ² ion in octahedral field, splitting of d ¹ to d ⁹ terms in an octahedral and tetrahedral field. Selection rules of d-d transitions. Vibronic and spin orbit coupling, effecting of weak to strong cubic fields on R-S terms, Comparison of CFSE values of d ¹ to d ⁹ ions in terms of orbit splitting and R-S term splitting. Orgel and Tanabe Sugano diagrams, Calculation of β and 10 Dq from spectral data. | 12 |
| III | Transition Metals Chemistry II: Molecular orbital theory-composition of ligand groups, orbitals, sigma and π -molecular | 11 |

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|----|---|----|
| | orbitals MOEL, diagrams of Oh, T _d and D _{4h} complexes with and without pi-bonds, charge transfer spectra. <i>Complexes of π-Acceptor Ligands:</i> π - acceptor character of CO, N ₂ , O ₂ , NO molecules in terms of MOEL diagrams, acid ligands of other groups of periodic table, Semi-bridging in metal carbonyls and isocyanides of metals. Magnetic, IR and X-ray diffraction evidence of their structure, acidity and softness, Symbiosis and anti-symbiosis, pi complexes of unsaturated organic molecules (bonding with C ₂ H ₄ only). Structures & the IR spectral properties representative transition metal carbonyl complexes | |
| IV | Magnetochemistry of Inorganic Compounds: Explanations of diamagnetism, paramagnetism, ferromagnetism and anti-ferromagnetism, origin of paramagnetic moment: electron spin moment, and orbital angular moment, magnetic susceptibility, Curie law, Curie-Weiss law, Bohr Magneton, magnetic susceptibility measurement using Gouy and Faraday methods, explanation of magnetic behaviours of transition metal complexes, Quenching of orbital angular momentum by crystal fields in complexes in terms of term-splitting. Effect of spin-orbit coupling and A, E & T states, Mixing in effect, first order and second order zeeman effects | 10 |

Reference Books

| S.No. | Author(s) | Title of the Book | Publisher/Year |
|-------|---|--|---|
| 1 | B.N. Figgis | Introduction to Ligand Fields, First Edition | John Wiley and Sons Ltd, United States (1999) |
| 2 | F.A. Cotton & G. Wilkinson, | Advanced Inorganic Chemistry, 3 rd Edition | John Wiley New York |
| 3 | F. Basolo and R.C. Johnson | Coordination Chemistry, 1 st Edition | W A Benjamin. INC, New York |
| 4 | J.E. Huheey, Ellen A. Keiter, Richard L. Keiter | Inorganic Chemistry, Principles of Structure and Reactivity, 4 th Edition | Harper Collins College Publishers |
| 5 | A.B.P. Lever | Inorganic Electronic-Spectroscopy, 2 nd Edition | Amsterdam, The Netherlands: Elsevier, 1984 |
| 6 | A. Earnshaw | Introduction to Magnetochemistry, 1 st Edition | Academic Press, London and New York |
| 7 | R.S. Drago | Physical Methods in Inorg. Chem., 1 st and 2 nd Edition | London, 1977 |

Course Outcomes and Mapping

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

CO1. Understand the fundamental concepts and postulates of various theories of coordination complexes.

CO2. Learn the stereochemistry and stability of the coordination complexes.

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|---|------|------|------|------|------|------|------|
| CO3. Derive spectroscopic terms for various electronic configurations and their correlation diagrams. CO4. Interpret electronic and magnetic properties of coordination compounds. CO5. Learn about the complexes of π -Acceptor ligands and analysis of their structural and spectral properties. | | | | | | | |
| | PSO1 | PSO2 | PSO3 | PSO4 | PSO5 | PSO6 | PSO7 |
| CO1 | 2 | 2 | 3 | 2 | 1 | 3 | 3 |
| CO2 | 2 | 3 | 4 | 3 | 1 | 3 | 2 |
| CO3 | 1 | 4 | 1 | 1 | 1 | 1 | 2 |
| CO4 | 2 | 2 | 2 | 1 | 4 | 2 | - |
| CO5 | 2 | 2 | - | - | 1 | 2 | - |

| I.K. GUJRAL PUNJAB TECHNICAL UNIVERSITY DEPARTMENT OF CHEMICAL SCIENCES | | | | |
|--|---|------------|------------|------------------|
| Course Name | M.Sc. Chemistry | | | |
| Subject Code: | CHL402-18 | | | |
| Subject Title: | REACTIVE INTERMEDIATES-I | | | |
| Contact Hours: | L:4 | T:0 | P:0 | Credits:4 |
| Examination Duration (hours) | 3 | | | |
| Objective(s): | 1. To predict the relationships between organic chemical structures and their reactivity. 2. To learn the fundamental and advanced concepts in reaction mechanisms in organic chemistry along with the study of reaction mechanisms in various types of substitution and elimination reactions. 3. To predict and account for the most commonly encountered reaction mechanisms in organic chemistry. | | | |

Details of the Course

| Unit | Contents | Contact Hours |
|-------------|--|----------------------|
| I | Reaction Mechanism: Structure and Reactivity: Type of mechanisms, types of reactions, thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammond's postulate, Curtin-Hammett principle, Potential energy diagrams, transition states and intermediates, methods of determining mechanisms, isotope effects. The Hammett equation and linear free energy relationship, substituent and reaction constants, Taft equation. Reactive intermediates: Formation and stability of Carbocations, Carbanions, Free Radicals, Carbenes, Nitrenes, and Arynes. Aromaticity: Huckel's rule and Concept of Aromaticity, Annulenes and Heteroannulenes, Fullerenes (C ₆₀). | 10 |
| II | Nucleophilic Substitution: Introduction, S _N 1 and S _N 2 Mechanism and evidence, Stereochemistry of nucleophilic substitution, Classical and nonclassical carbocations, phenonium ions, norbornyl system, common carbocation rearrangements, Ambient Nucleophiles, SET Mechanism, Neighboring Group Participation reaction (NGP). The S _N i mechanism, mixed S _N 1 and S _N 2 Reactions, Effect of substrate structure; attacking nucleophile; leaving group and reaction medium in S _N 1 and S _N 2 reactions, phase-transfer catalysis, regioselectivity. Nucleophilic Substitution of allylic systems Nucleophilic displacements at Allylic halides/tosylates, Benzylic position, allylic, aliphatic trigonal and a vinylic carbon, & Aryl halide. Nucleophilic aromatic substitution: Nucleophilic aromatic substitution by addition-elimination mechanism and Elimination addition mechanism (S _N Ar, S _N 1, benzyne and S _{RN} 1 mechanisms), effect of substrate, structure, leaving group and attacking | 13 |

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|-----|--|----|
| | nucleophile, Von Richter, Sommelet-Hauser, and Smiles rearrangements. | |
| III | <p>Electrophilic Substitutions: Introduction, Different mechanism for aliphatic electrophilic substitution (Bimolecular mechanisms-SE₂ and SE_i The SE₁ mechanism), Electrophilic Substitution accompanied by double bond shift, Aliphatic Electrophilic Substitution in relation to substrate structure, Leaving group & solvent polarity, Effect of substrates, leaving group and the solvent polarity on the reactivity,</p> <p>Aromatic electrophilic substitution: Structure-Reactivity relationship: arenium ion mechanism; orientation and reactivity in mono substitution and disubstituted aromatics; energy profile diagram; the ortho/para ratio; ipso attack; orientation in different ring systems; quantitative treatment of reactivity in substrates and electrophiles; Diazo coupling, Vilsmeier reaction, Gatterman-Koch reaction, Beckmann reaction, Hoesch reaction.</p> | 12 |
| IV | <p>Free Radical Substitution: Types of free radical reactions, free radical substitution mechanism, mechanism at an aromatic substrate, neighbouring group assistance. Reactivity for aliphatic and aromatic substrates at a bridgehead, Reactivity in the attacking radicals. The effect of solvents on reactivity. 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.</p> <p>Elimination Reactions: E₁, E₂ and E_{1c}b mechanisms - E₁, E₂ and E_{1c}B spectrum, Regiochemistry and stereochemistry of elimination reactions, Orientation of the double bond, Hoffman and Saytzeff rules, Competition between elimination and substitution. Typical eliminations reactions - dehydration, dehydrohalogenation and dehalogenation. Stereochemistry of E₂ eliminations in cyclohexane systems. Mechanism of pyrolytic eliminations. Chugaev and Cope eliminations.</p> | 10 |

Reference Books

| S.No. | Author(s) | Title of the Book | Publisher |
|-------|--|--|--|
| 1 | Francis A. Carey and Richard J. Sundberg | Advanced Organic Chemistry Vol. A and Vol. B, fourth Edition | Kluwer Academic publishers, New York 2002 |
| 2 | Jerry March | Organic Reaction Mechanism | John Wiley Ed. 5, 2002 |
| 3 | W. Carruthers | Some Modern Methods of Organic Synthesis, IV Edition | Cambridge University Press, 2004 |
| 4 | H.O. House | Modern Synthetic Reactions | The Benjamin Cummings Publishing Company, London, 1972 |
| 5 | R.O.C. Norman | Principles of organic synthesis | Chapman and Hall, London. 1980 |
| 6 | John McMurry and Eric Simanek | Fundamentals of Organic Chemistry | Cengage Learnings |

| | | | |
|---|---------------------------------|-------------------------------|--|
| 7 | T.L. Gilchrist and C.W. Rees | Carbenes, Nitrenes and Arynes | Thomas Nelson and Sons Ltd., London |
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Course Outcomes and Mapping

At the end of the course, the student will be able

- CO1.** to study the various known reactive intermediate in organic synthesis
- CO2.** to predict the relationships between organic chemical structures and their reactivity.
- CO3.** to learn the fundamental and advanced concepts in reaction mechanisms in organic chemistry along with the study of reaction mechanisms in various types of substitution and elimination reactions.
- CO4.** to study the new methodologies for altering the reactivity patterns of reactive intermediates
- CO5.** to synthesize various molecules using combinations of reactive intermediates

| | PSO1 | PSO2 | PSO3 | PSO4 | PSO5 | PSO6 | PSO7 |
|-----|------|------|------|------|------|------|------|
| CO1 | 2 | 3 | 4 | 1 | ... | 3 | 2 |
| CO2 | 1 | 3 | 4 | 1 | 3 | 2 | 2 |
| CO3 | 1 | 3 | 3 | 1 | ... | 2 | 3 |
| CO4 | 1 | 4 | 4 | 1 | 1 | 3 | 2 |
| CO5 | 2 | 4 | 2 | 1 | 1 | 3 | 2 |

| I.K. GUJRAL PUNJAB TECHNICAL UNIVERSITY DEPARTMENT OF CHEMICAL SCIENCES | | | | |
|--|---|------------|------------|------------------|
| Course Name | M.Sc. Chemistry | | | |
| Subject Code: | CHL403-18 | | | |
| Subject Title: | PHYSICAL CHEMISTRY-I | | | |
| Contact Hours: | L:4 | T:0 | P:0 | Credits:4 |
| Examination Duration (hours) | 3 | | | |
| Objective(s): | This course will equip students with the necessary chemical knowledge concerning the fundamentals in the basic areas of physical chemistry viz. thermodynamics, electrochemistry and chemical kinetics, with regard to various theories developed and their applicability for various systems under consideration. The problem solving skills of students are expected to be enhanced through due weightage given to numerical problems in each unit. | | | |

Details of the Course

| Unit | Contents | Contact Hours |
|-------------|--|----------------------|
| I | Classical Thermodynamics: Brief introduction, partial molar properties; partial molar free energy, chemical potential, partial molar volume, partial molar heat content and their significance. Gibbs-Duhem equation. Determination of partial molar volume by method of intercept. Concept of fugacity and determination of fugacity in liquids and gases. Non-ideal solutions; activity and activity coefficient, Debye-Huckel theory for activity coefficient of electrolytic solutions, Determination of activity and activity coefficients, ionic strength, Numerical Problems. | 10 |
| II | Electrochemistry-I: Electrolytic conductance and its measurement; Kohlrausch's Law and its applications; Conductometric titrations, Anomaly of strong electrolytes, Debye-Huckel theory, Onsager equation and its verification, Debye-Falkenhagen effect, Wien effect, Thermodynamics of electrified interface equation, Derivation of electrocapillary, Lippmann equation. Structure of electrified interfaces, Electrical double layer, Theories of structure of electrical double layer: Helmholtz-Perrin model, Gouy-Chapman model and Stern model. Polarography: Ilkovic equation and its derivation, concentration polarization, instrumentation, advantages of DME, half wave potential, Applications of polarography. Numericals. | 13 |
| III | Chemical Dynamics: Collision theory, modified collision theory, weakness of the collision theory, theory of absolute reaction rates, equilibrium hypothesis, Derivation of the rate equation, statistical mechanical derivation and thermodynamic formulation. Isotope effect on reaction rate; Primary isotope effect, secondary isotope effect. Dynamics of unimolecular reactions; Lindemann, Hinshelwood and RRKM theories for unimolecular reactions. | 12 |

| | | |
|----|--|----|
| IV | Kinetics of Reactions: Kinetics of Complex Reactions; Opposing Reactions, Consecutive reactions, Chain Reactions. Kinetics of reactions in solution: Reaction between ions, influence of solvent-double sphere model, single sphere model, influence of ionic strength. Kinetics of fast reactions; Flow methods for study of fast reactions, pulse methods, flash photolysis and NMR method. Numericals. | 10 |
|----|--|----|

Reference Books

| S.No. | Author(s) | Title of the Book | Publisher/Year |
|-------|---------------------------|---|--------------------------------------|
| 1 | P.W. Atkins | Physical Chemistry, 3 rd edition | ELBS (1987) |
| 2 | S.H. Maron & C.F. Prutton | Principles of Physical Chemistry, 1 st edition | Oxford and IBH (1958) |
| 3 | G.W. Castellan | Physical Chemistry, 4 th edition | Narosa (2004) |
| 4 | S. Glasstone | Thermodynamics for Chemists | Affiliated East-West Press Pvt. Ltd. |
| 5 | S. Glasstone | An introduction to Electrochemistry | Affiliated East-West Press Pvt. Ltd. |
| 6 | K.J. Laidler | Chemical kinetics | Harper and Row, New York (1987) |
| 7 | D.R. Crow | Principles and Applications of Electro-chemistry | Blackie academic, Glasgow (1988) |

Course Outcomes and Mapping

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

- CO1.** Understand the basic principles and theories pertaining to thermodynamics, electrochemistry and chemical kinetics.
- CO2.** Solve various problems related to non ideal systems.
- CO3.** Define the dynamics of various types of reactions.
- CO4.** Familiar with the various techniques used for determination of rates of reactions.
- CO5.** Rationalise bulk properties and processes using thermodynamic considerations.
- CO6.** Apply the concepts related to conductance in solving problems related to electrolytes.

| | PSO1 | PSO2 | PSO3 | PSO4 | PSO5 | PSO6 | PSO7 |
|-----|------|------|------|------|------|------|------|
| CO1 | 2 | 4 | 5 | 3 | ... | 2 | 4 |
| CO2 | 2 | 5 | 5 | 2 | 3 | 2 | 5 |
| CO3 | 2 | 2 | 3 | 2 | 1 | 1 | 2 |
| CO4 | 2 | 2 | 2 | 3 | 4 | 2 | 2 |
| CO5 | 2 | 4 | 5 | 3 | ... | 2 | 4 |
| CO6 | 2 | 5 | 5 | 2 | 3 | 2 | 5 |

| I.K. GUJRAL PUNJAB TECHNICAL UNIVERSITY DEPARTMENT OF CHEMICAL SCIENCES | | | | |
|--|---|------------|------------|------------------|
| Course Name | M.Sc. Chemistry | | | |
| Subject Code: | CHL404-18 | | | |
| Subject Title: | SPECTROSCOPY-I | | | |
| Contact Hours: | L:4 | T:0 | P:0 | Credits:4 |
| Examination Duration (hours) | 3 | | | |
| Objective(s): | 1. To learn various techniques of spectrometric identification of organic compounds 2. To characterize organic compounds by applying various techniques together | | | |

Details of the Course

| Unit | Contents | Contact Hours |
|------|--|---------------|
| I | General Features of Spectroscopy: Introduction to spectroscopy, Nature of radiation, Energies corresponding to various kinds of radiation, Experimental techniques, intensities of spectral lines, Selection rules and transition moments, Line widths, Broadening. UV and Visible Spectroscopy of organic molecules: Measurement techniques, Beer – Lambert's Law, molar extinction coefficient, oscillator strength and intensity of the electronic transition, Frank Condon Principle, Ground and first excited electronic states of diatomic molecules, relationship of potential energy curves to electronic spectra, Chromophores, auxochromes, blue shift, red shift, hypsochromic and bathochromic effect, $\sigma\text{-}\sigma^*$, $\pi\text{-}\pi^*$, $n\text{-}\pi^*$ transitions in organic molecules, Woodward rules for conjugated dienes and α , β -unsaturated carbonyl groups, extended conjugation and aromatic sterically hindered systems, Quantitative applications. | 10 |
| II | Infrared Spectroscopy: Introduction, Principle of IR spectroscopy, modes of vibrations, Vibrational frequency, fundamental vibrations, Selection rules, factors affecting vibrational frequencies, IR spectrophotometer, sampling techniques, special features of different classes of organic compounds pertaining to IR spectroscopy (such as aliphatic and aromatic hydrocarbons, halogen compounds, alcohols and phenols, ethers, carbonyl compounds, acids and its derivatives, amines and amides, nitro and nitrides, nitrile compounds, heteroaromatic compounds etc.) and interpretation of IR spectrum, quantitative applications. | 10 |
| III | Nuclear Magnetic Resonance Spectroscopy: PMR: Natural abundance of ^{13}C , ^{19}F and ^{31}P nuclei; The spinning nucleus, effect of external magnetic field, precessional motion and frequency, Energy transitions, Chemical shift and its measurements. Factors influencing chemical shift, anisotropic effect; Integrals of protons, proton exchange, spin-spin coupling- splitting theory, one, two and three bond coupling, virtual, long range and allylic coupling, magnitude of coupling constant; factors affecting the coupling constant, Chemical | 15 |

| | | |
|----|---|----|
| | and magnetic equivalence, First and second order spectra, A2, AB, AX, AB2, AX2, A2B2 and A2X2 spin systems, Simplification of complex spectra (solvent effect, field effect, double resonance and lanthanide shift reagents), CW and FT NMR, Relaxation processes, T1 and T2 measurements, Applications of PMR in structural elucidation of simple and complex compounds. ¹³C-NMR: Resolution and multiplicity of ¹³ C NMR, ¹ H-decoupling, noise decoupling, broad band decoupling; Deuterium, fluorine and phosphorus coupling; NOE and origin of nuclear overhauser effect. off-resonance, proton decoupling, Structural applications of ¹³ C-NMR., pulse sequences, pulse widths, spins and magnetization vectors, DEPT, INEPT, Introduction to 2D-NMR, COSY, NOESY, HMBC and HSQC spectra. | |
| IV | Mass Spectrometry: Introduction, methods of ionization EI & CI, Brief description of LD, FAB, SIMS, FD etc., Ion analysis methods (in brief), isotope abundance, Metastable ions, general rules predicting the fragmentation patterns. Nitrogen rule, determination of molecular ion peak, index of H efficiency, fragmentation patterns for aliphatic compounds, alkyl halides, aryl halides, alcohols, amines, aldehydes, Ketones, esters, amides, nitriles, carboxylic acids, ethers, monocyclic aromatic compounds. | 10 |

Reference Books

| S.No. | Author(s) | Title of the Book | Publisher/Year |
|-------|--|--|----------------------------|
| 1 | Donald L. Pavia, Gary M. Lampman, George S. Kriz & James R. Vyvyan | Spectroscopy | Cengage learnings |
| 2 | Robert. M. Silverstein, Francis X. Webster, David J. Kiemle & David L. Bryce | Spectrometric Identification of Organic Compounds. | Wiley, 2007 |
| 3 | W. Kemp | Organic Spectroscopy | Palgrave Macmillan |
| 4 | D.H. Williams, I. Fleming | Spectroscopic Methods in Organic Chemistry | New Age International |
| 5 | R. F. Barrow, Derek A. Long, D. J. Millen | Molecular Spectroscopy | Royal Society of Chemistry |
| 6 | C.N Banwell | Fundamentals of Molecular Spectroscopy | Tata Mc Graw Hill |

Course Outcomes and Mapping

| | |
|---|---|
| At the end of the course, the student will be able to | |
| CO1. | Solve structural problems based on UV-Vis, IR, ¹ H-NMR, ¹³ C-NMR and mass spectral data. |
| CO2. | Elucidate the structures of various organic compounds on the basis of spectral data. |
| CO3. | Understand various involved processes responsible for NMR chemical shifts and splitting patterns and mass spectrometry. |
| CO4. | Illustrate the mechanisms that give rise to the infrared and UV-Visible absorption bands and identify to which functional groups each correspond. |

| | | | | | | | |
|-----|------|------|------|------|------|------|------|
| | | | | | | | |
| | PSO1 | PSO2 | PSO3 | PSO4 | PSO5 | PSO6 | PSO7 |
| CO1 | 3 | 5 | 3 | 1 | 5 | 4 | 2 |
| CO2 | 3 | 4 | 3 | - | 5 | 3 | 2 |
| CO3 | 2 | 4 | 3 | - | 4 | 2 | 2 |
| CO4 | 3 | 4 | 3 | 2 | 3 | 2 | 2 |

| I.K. GUJRAL PUNJAB TECHNICAL UNIVERSITY DEPARTMENT OF CHEMICAL SCIENCES | | | | |
|--|--|-----|-----|-----------|
| Course Name | M.Sc. Chemistry | | | |
| Subject Code: | CHL405-18 | | | |
| Subject Title: | ENVIRONMENTAL CHEMISTRY | | | |
| Contact Hours: | L:3 | T:0 | P:0 | Credits:3 |
| Examination Duration (hours) | 3 | | | |
| Objective(s): | The specialisation in “Environmental Chemistry,” gives an insight to the role of various environmentally harmful substances for the degradation of the environment. The students will learn what is toxic, and most importantly, will become an expert on what we can do to find solutions to the challenges of toxic substances in the environment. | | | |

Details of the Course

| Unit | Contents | Contact Hours |
|------|--|---------------|
| I | <p>Air Pollution: Chemical composition of atmosphere- particles, ions and radicals and their formation, Sources and sinks of gases pollutants, classification & effects of air pollutants on living and nonliving things, Air pollution problems in India, pollution problems in industrial area, global air pollution problems, smog, green house effect, global warming, acid rain, ozone depletion and their consequences on Environment. Major air pollution disasters.</p> <p>Water pollution: Chemical composition of water bodies-lakes, streams, rivers and wet lands, Types, sources and classification of water pollutants, Industrial water pollution, constituents of aquatic Environment, oxygen contents of water and aquatic life, oxygen electrode, and its use, mercury pollution and estimation of organo-mercurials, Effects of water pollutants on life and Environment.</p> | 4 4 |
| II | Analysis of air and water pollutants: Water analysis: Color, odour, conductivity, TDS, pH, acidity, alkalinity, chloride, residual chlorine, hardness, trace metal analysis, elemental analysis, ammonia, nitrite, nitrate, fluoride, sulphide, phosphate, phenols, surfactants, BOD, COD, DO, TOC, non-dispersive IR spectroscopy, anode stripping, ICP, AES, Chromatography, ion-selective electrodes, neutron activation analysis. | 12 |
| III | Soil pollution: Soil humus, soil fertility, inorganic and organic components in soil, acid-base and ion exchange reactions in soils, micro and macro nutrients, wastes and pollutants in soil, introduction to geochemistry, treatment and recycling soil analysis, radioactive pollution, disposal of radioactive waste. Pesticide, residue analysis soil pollution, Sources of pesticides residue in the Environment, pesticides degradation by natural forces, effect of | 12 |

| | | |
|----|---|----|
| | pesticide residue on life, Analytical techniques (HPLC, GC-MS) for pesticides residue analysis. | |
| IV | Radiation pollution: Classification & effects of radiation, effects of ionizing radiation on man, Effects of non ionizing radiation on life, radioactivity and Nuclear fall out, protection and control from radiation. Environmental toxicology, chemical solutions to environmental problems, biodegradability, principles of decomposition, better industrial processes, Bhopal gas tragedy, Chernobyl, three mile island, sewozo and minamata disasters. | 13 |

Reference Books

| S.No. | Author(s) | Title of the Book | Publisher/Year |
|-------|--------------------------------|---|-----------------------------|
| 1 | A.K. De | Environmental Pollution | Wiley Eastern |
| 2 | Wark & Werner | Air Pollution | IEP |
| 3 | S.P. Mahajan | Environmental Pollution Control in Process Industries | Tata Mc-graw Hill Education |
| 4 | B.K. Sharma & H.Kaur | Environmental Pollution | Krishna |
| 5 | P.K. Trivedi | Introduction to Air Pollution | |
| 6 | S.M. Khopkar | Environmental Pollution Analysis | Wiley Eastern |
| 7 | F. J. Welcher | Standard method of chemical analysis | Van-Nostrand Reinhold |
| 8 | B.K. Sharma & H.Kaur | Environmental Chemistry | Krishna |
| 9 | T. D. Biswas & S. K. Mukherjee | Text book of soil science | Tata Mc-graw Hill Education |

Course Outcomes and Mapping

| | | | | | | | |
|---|---|------|------|------|------|------|------|
| At the end of the course, the student will be able to | | | | | | | |
| CO1. | Acquire fundamental knowledge and understanding of the physical environment (land, water, air and climate) and will develop insights into key concepts in the field of environmental Chemistry. | | | | | | |
| CO2. | Understand the basic phenomena of atmospheric sciences, hydrology of different aquatic ecosystems and soil science. | | | | | | |
| CO3. | Develop sound theoretical background of basic chemistry associated with toxicology of environmental pollutants | | | | | | |
| CO4. | Get acquainted with the sources, properties and ill-effects of important air, water, soil and radioactive pollutants in air, water and soil and apply analytical tools to determine and measure pollutants in various environmental samples | | | | | | |
| CO5. | Become aware of the local, regional and global environmental problems. | | | | | | |
| | PSO1 | PSO2 | PSO3 | PSO4 | PSO5 | PSO6 | PSO7 |
| CO1 | 3 | 4 | 3 | 2 | 3 | 4 | 4 |
| CO2 | 2 | 3 | 3 | 3 | 2 | 3 | 5 |
| CO3 | 3 | 3 | 3 | 2 | 2 | 2 | 3 |
| CO4 | 3 | 5 | 3 | 4 | 4 | 4 | 3 |
| CO5 | 3 | 1 | 2 | 5 | 2 | 2 | 3 |

| I.K. GUJRAL PUNJAB TECHNICAL UNIVERSITY DEPARTMENT OF CHEMICAL SCIENCES | | | | |
|--|---|------------|------------|------------------|
| Course Name | M.Sc. Chemistry | | | |
| Subject Code: | CHL406A-18 | | | |
| Subject Title: | HUMAN PHYSIOLOGY | | | |
| Contact Hours: | L:3 | T:0 | P:0 | Credits:3 |
| Examination Duration (hours) | 3 | | | |
| Objective(s): | Chemistry has its large applications in Human functioning. Most of the important functions that a human body performs from molecular to organ system level follows the basic principles of Chemistry & Physics. Therefore the major objective of teaching this subject is to understand the various chemical functions which involve mechanisms underlying communication & coordination within an organism and to elucidate the structure of various parts in relationship with its functions to bring about homeostasis within the body. | | | |

Details of the Course

| Unit | Contents | Contact Hours |
|------|---|---------------|
| I | Introduction : General Introduction to anatomy, physiology and its related sciences. Physico-chemical laws and their applications in Physiology. Elementary Composition of a Human Body Cell Structure and Functions- A Basis of Physiology: Structure and functions of subcellular organelles, Elementary tissues (Epithelial, Muscular, Connective & Nervous) of the Human Body, their structure & functions, molecular mechanism of skeletal muscle contraction, nerve conduction, membrane transport and cell division | 2 8 |
| II | Digestive System: Physiological anatomy and histology of the digestive system, Functions of Digestive system, Digestive juices (Saliva, Gastric, Pancreatic Bile and Intestinal), their composition, functions and mechanism of secretions, movements of alimentary canal and gut reflexes, digestion of carbohydrates, proteins, lipids and their absorption Vitamins: History, characteristics, composition and functions of various vitamins (Vitamins A, D, E, K, C B ₁ , B ₂ , B ₃ B ₆ and B ₁₂) etc. | 8 2 |
| III | Cardiovascular System: Systemic & Pulmonary Circulation; Hepatic, Renal & Hypophyseal portal circulation. Anatomy of Heart and properties of cardiac muscles. Origin and conduction of Heart beat. Nervous & chemical regulation of Heart beat. Cardiac | 8 |

| | | |
|----|--|------------|
| | cycle, heart sounds, ECG, Cardiac output. Blood pressure and its regulation. Respiratory System: Anatomy of respiratory system, mechanism of pulmonary ventilation, pulmonary volumes and lung capacities, physical principles and mechanisms of gaseous exchange and transport, regulation of respiration. | 6 |
| IV | Excretory System: Physiological anatomy of the kidneys and urinary tract, urine formation (glomerular filtration, tubular reabsorption and secretion) and its regulation. Endocrine System: Introduction and General Mechanisms of physiological action of Pituitary hormones, Thyroid hormones, Adrenocortical hormones, Pancreatic hormones, Parathormone and Calcitonin, Gonadal hormones. | 5 6 |

Reference Books

| S.No. | Author(s) | Title of the Book | Publisher/Year |
|-------|--------------------------------------|---|---|
| 1. | Anne Waugh & Alison Grant | Ross & Wilson Human Anatomy & Physiology | Churchil Livingstone Elsevier Publishers, China. 2014 |
| 2. | C.C. Chatterjee | Human Physiology Vol. I & II | Medical Allied Agency, Calcutta. 2000 |
| 3. | A.C. Guyton & J.E. Hall | Textbook of Medical Physiology. 9 th edition | Prism Book Pvt Ltd. India. 1996 |
| 4. | Gerard G. Tortora & Bryan Derrickson | Principles of Anatomy & Physiology. 12 th edition. | John Wiley & Sons, USA. 2009 |

Course Outcomes and Mapping

| | | | | | | | |
|---|---|------|------|------|------|------|------|
| At the end of the course, the student will be able to | | | | | | | |
| CO1. | Understand basic structure and functioning of human organs. | | | | | | |
| CO2. | Learn various physiological processes to understand functioning of important organ systems. | | | | | | |
| CO3. | Know how various organs bring about homeostasis. | | | | | | |
| CO4. | Describe the relationship between structure & functions of cells, tissues & organs. | | | | | | |
| CO5. | Understand how the hormones effect the working of whole body organs. | | | | | | |
| | PSO1 | PSO2 | PSO3 | PSO4 | PSO5 | PSO6 | PSO7 |
| CO1 | 2 | - | 1 | - | 1 | 3 | 2 |
| CO2 | 3 | - | 3 | - | 1 | 4 | 3 |
| CO3 | 3 | | 2 | 1 | 1 | 4 | 2 |
| CO4 | - | 2 | 1 | 1 | 1 | 2 | 2 |
| CO5 | 3 | 2 | 3 | 1 | 1 | 3 | 3 |

| I.K. GUJRAL PUNJAB TECHNICAL UNIVERSITY DEPARTMENT OF CHEMICAL SCIENCES | | | | |
|--|--|------------|------------|------------------|
| Course Name | M.Sc. Chemistry | | | |
| Subject Code: | CHL406B-18 | | | |
| Subject Title: | NUMERICAL METHODS FOR CHEMISTS | | | |
| Contact Hours: | L:3 | T:0 | P:0 | Credits:3 |
| Examination Duration (hours) | 3 | | | |
| Objective(s): | To make students familiar with the basic concepts of mathematics for understanding theoretical treatments and solving numerical problems in other courses being taught in the class. | | | |

Details of the Course

| Unit | Contents | Contact Hours |
|------|--|---------------|
| I | Matrix Algebra: Addition and multiplication; inverse, adjoint and transpose of matrices, special matrices (Symmetric, skew-symmetric, Hermitian, skew-hermitian, unit, diagonal, unitary etc.) and their properties. Matrix equations: Homogeneous, non- homogeneous linear equations and introduction to vector spaces, matrix eigenvalues, diagonalization, determinants (examples from Huckel theory). | 11 |
| II | Differential Calculus: Functions, continuity and differentiability, applications of differential calculus including maxima and minima (examples related to maximally populated rotational energy levels, Bohr's radius and most probable velocity from Maxwell's distribution etc), exact and inexact differentials with their applications to thermodynamic properties. Integral calculus, basic rules for integration, integration by parts, partial fraction and substitution. Reduction formulae, applications of integral calculus. Functions of several variables, partial differentiation, co- ordinate transformations (e.g. Cartesian to spherical polar). | 12 |
| III | Elementary Differential Equations: Variables-separable and exact first-order differential equations, homogeneous, exact and linear equations. Applications to chemical kinetics, secular equilibria, quantum chemistry etc. Solutions of differential equations by the power series method, order differential equations and their solutions. | 11 |

| | | |
|----|--|----|
| IV | Permutation and Probability: Permutations and combinations, probability and probability theorems, average, root mean square and most probable errors, examples from the kinetic theory of gases etc, curve fitting (including least squares fit etc) with a general polynomial fit. | 11 |
|----|--|----|

Reference Books

| S.No. | Author(s) | Title of the Book | Publisher/Year |
|-------|-----------------------|---|-------------------------|
| 1 | E.Steiner | The Chemistry Mathematics Book | Oxford University Press |
| 2 | Doggett and Sutcliffe | Mathematics for Chemistry | Longman |
| 3 | F. Daniels | Mathematical Preparation for Physical Chemistry | McGraw Hill |
| 4 | D.M. Hirst | Chemical Mathematics | Longman |
| 5 | J.R. Barrante | Chemical Mathematics for Physical Chemistry | Prentice Hall |
| 6 | Tebbutt | Basic Mathematics for Chemist | Wiley |

Course Outcomes and Mapping

| | | | | | | | |
|---|--|------|------|------|------|------|------|
| At the end of the course, the student will be able to | | | | | | | |
| CO1. | Learn the use of derivatives in chemistry is when they want to find the concentration of an element in a product. Differentiation is used to calculate rate of reaction and compressibility in chemistry. | | | | | | |
| CO2. | Understand the various basic mathematical methods for chemists. The methods involve matrices, differentiation, integration, first and second order differential equations and their solutions. | | | | | | |
| CO3. | Students will be able to explore the idea how to use basic math, probability in chemistry to enhance the physical chemistry courses like quantum mechanics and statistics mechanics. | | | | | | |
| CO4. | Develop understanding and fluency in mathematics through inquiry, exploring and connecting mathematical concepts in chemistry and applying problem-solving skills and mathematical techniques. The theory of matrices which are used in solving equations related to chemical reactions. | | | | | | |
| CO5. | Develop the ability to use a variety of representations, in written, graphical form, to formulate and express mathematical ideas. They will communicate mathematically terminology and notations. | | | | | | |
| CO6. | Understand the concept of permutations and combinations during defining of structures of reactions. Applications of differential equations as chemical kinetics, secular equilibria, quantum chemistry. | | | | | | |
| | PSO1 | PSO2 | PSO3 | PSO4 | PSO5 | PSO6 | PSO7 |
| CO1 | 4 | 4 | 2 | 4 | 3 | 3 | 2 |
| CO2 | 3 | 3 | 4 | 2 | 3 | 4 | 3 |
| CO3 | 4 | 5 | 3 | 2 | 2 | 3 | 2 |

| | | | | | | | |
|-----|---|---|---|---|---|---|---|
| CO4 | 4 | 4 | 4 | 3 | 4 | 5 | 5 |
| CO5 | 4 | 3 | 3 | 3 | 4 | 4 | 3 |
| CO6 | 5 | 2 | 4 | 3 | 5 | 4 | 3 |

| I.K. GUJRAL PUNJAB TECHNICAL UNIVERSITY DEPARTMENT OF CHEMICAL SCIENCES | | | | |
|--|---|------------|------------|------------------|
| Course Name | M.Sc. Chemistry | | | |
| Subject Code: | CHP407-18 | | | |
| Subject Title: | INORGANIC CHEMISTRY LAB | | | |
| Contact Hours: | L:0 | T:0 | P:6 | Credits:3 |
| Examination Duration (hours) | 6 | | | |
| Objective(s): | The objective of this course is to provide practical knowledge and illustrative experiments about synthesis and characterization of inorganic complexes and estimation of metal ions. | | | |

Details of the Course

| Unit | Contents |
|------|---|
| I | <p>Synthesis and characterization of following complexes and estimation of metal ions:</p> <ol style="list-style-type: none"> 1. Synthesis of tris(ethylenediamine)nickel(II) dichloride, $[\text{Ni}(\text{en})_3]\text{Cl}_2$, and estimation of Ni(II). Record and interpret its IR, UV-vis and magnetic susceptibility. 2. Synthesis of hexaaminenickel(II) dichloride $[\text{Ni}(\text{NH}_3)_6]\text{Cl}_2$ and estimation of Ni(II). Record and interpret its IR, UV-vis and magnetic susceptibility. 3. Synthesis of $[\text{Cu}(\text{NH}_3)_4]\text{SO}_4 \cdot \text{H}_2\text{O}$ and estimation of Copper. 4. To prepare cis and trans copper glycine complexes. 5. Preparation of $[\text{VO}(\text{acac})_2]$. Record and interpret its IR, UV-vis and magnetic susceptibility. 6. To prepare a pure sample of tris(acetylacetonate)cobalt(III), $\text{Co}(\text{acac})_3$. Record and interpret its IR, UV-vis spectrum. 7. Preparation of tris(nitro-acetylacetonate)cobalt(III), $\text{Co}(\text{acac}-\text{NO}_2)_3$, record and interpret its proton NMR spectrum. 8. To prepare $[\text{Fe}(\text{NO})(\text{S}_2\text{CNEt}_2)_2]$. Record and interpret its IR and UV-vis spectrum, Magnetic Susceptibility and Analysis of Fe(II). |
| II | <p>Gravimetric Analysis</p> <ol style="list-style-type: none"> 1. Determination of Ba^{2+} as its chromate. 2. Estimation of lead as its lead molybdate. 3. Estimation of chromium (III) as its lead chromate. 4. Estimation of Cu^{2+} using Ammonium/Sodium thiocyanate |

Reference Books

| S.No. | Author(s) | Title of the Book |
|-------|--|---------------------------------|
| 1 | J.R. Barrante G. Marr and B.W. Rockett | Practical Inorganic Chemistry |
| 2 | Vogel | Inorganic Quantitative Analysis |

Course Outcomes and Mapping

| | | | | | | | |
|--|------|------|------|------|------|------|------|
| At the end of the course, the students will learn | | | | | | | |
| CO1. Preparation of different inorganic complexes. | | | | | | | |
| CO2. Purification and crystallisation of inorganic compounds. | | | | | | | |
| CO3. Interpretation of compounds using UV-Vis, FT-IR techniques. | | | | | | | |
| CO4. Measurement of various physical properties such as magnetic moment of complexes. | | | | | | | |
| CO5. Gravimetric analysis of various cations. | | | | | | | |
| | PSO1 | PSO2 | PSO3 | PSO4 | PSO5 | PSO6 | PSO7 |
| CO1 | 5 | 1 | 4 | 2 | 5 | 2 | - |
| CO2 | 5 | 1 | 4 | 1 | 5 | 2 | - |
| CO3 | 5 | 4 | 5 | - | 5 | 3 | 4 |
| CO4 | 3 | 4 | 5 | - | 4 | 2 | 2 |
| CO5 | 5 | 2 | 2 | - | 5 | 1 | - |

| I.K. GUJRAL PUNJAB TECHNICAL UNIVERSITY DEPARTMENT OF CHEMICAL SCIENCES | | | | |
|--|--|------------|------------|------------------|
| Course Name | M.Sc. Chemistry | | | |
| Subject Code: | CHP408-18 | | | |
| Subject Title: | ORGANIC SYNTHESIS LAB | | | |
| Contact Hours: | L:0 | T:0 | P:6 | Credits:3 |
| Examination Duration (hours) | 6 | | | |
| Objective(s): | 1. To learn various practical techniques for synthesis, identification, isolation, purification and characterization of organic compounds. 2. To carry out hand on experience the various methods of organic synthesis. | | | |

Details of the Course

| Unit | Contents |
|------|--|
| I | Techniques: (At least One Practical of Each Technique) Crystallization, Purification by Sublimation, Distillation, Fractional Distillation, Steam Distillation, Vacuum Distillation, Preparative chromatography, Column Chromatography, TLC stains preparation and Thin Layer Chromatography. (Purity is to be checked by m.p. and mixed m.p.) |
| II | Preparation of Derivatives: (Each Derivative of at least one Compound) Oxime, 2,4-DNP, Acetyl, Benzoyl, Semicarbazone, Anilide, Amide, Aryloxyacetic acid. |
| III | Preparations: (a) At least eight single stage preparations from the following should be carried out. The preparations should be carried out on micro scale. i) Cyclohexanone to Adipic acid ii) Benzophenone to Benzhydral iii) Anthracene to Anthraquinone iv) Chlorobenzene to 2,4-Dinitrochlorobenzene v) 2,4-Dinitrochlorobenzene to 2,4-Dinitrophenol vi) Acetoacetic ester to 1-Phenyl-3-methyl-5 pyrazolone vii) Benzaldehyde to Cinnamic acid viii) 4-Chlorobenzaldehyde to 4-Chlorobenzoic acid and 4-Chlorobenzyl alcohol ix) Benzene to β -Benzoyl propionic acid x) Benzaldehyde to Dibenzylidene acetone xi) p-Aminobenzoic acid to p-Chlorobenzoic acid xii) N,N-Dimethylaniline to 4-Formyl-N, N-dimethyl aniline xiii) Benzophenone to Benzpinacol xiv) p-Nitrotoluene to p-Nitro benzoic acid |

| | |
|--|---|
| | xv) Anisole to 2,4-Dinitroanisole xvi) Phthalic anhydride to phthalimide xvii) Phthalimide to Anthranilic acid xviii) Acetanilide to p-Bromoacetanide xix) p-Bromoacetanide to p-Bromoaniline xx) m-Dinitrobenzene to m-Nitroaniline (b) Minimum 2 two stage and 2 three stage preparations to reveal how to develop a synthetic sequence. (c) Interpretation of NMR, IR and Mass Spectra of about 10 compounds. |
|--|---|

Reference Books

| S.No. | Author(s) | Title of the Book | Publisher |
|-------|--|--|-------------------|
| 1 | Brian S. Furniss, Antony J. Hannaford, Peter W.G. Smith and Austin R. Tatchell | Vogel's Textbook of Practical Organic Chemistry, 5 th Edition | Longman, London |
| 2 | F.G. Mann and B. C. Saunders | Practical Organic Chemistry | Longman, New York |
| 3 | John Leonard, Barry Lygo and Garry Procter | Advanced Practical Organic Chemistry, Third Edition | CRC Press, London |
| 4 | J.T. Sharp | Practical Organic Chemistry: A student handbook of techniques | Springer |
| 5 | Philippa B. Cranwell, Laurence M. Harwood and Cristopher J. Moody | Experimental Organic Chemistry, 3 rd Edition | Wiley |
| 6 | Robert. M. Silverstein, Francis X. Webster, David J. Kiemle & David L. Bryce | Spectrometric Identification of Organic Compounds. | Wiley, 2007 |

Course Outcomes and Mapping

| | | | | | | | |
|--|---|------|------|------|------|------|------|
| At the end of the course, the students will be able to | | | | | | | |
| CO1. | Apply various methods techniques in organic synthesis to build organic molecules. | | | | | | |
| CO2. | Understand the fundamental mechanistic pathways of organic synthesis involving various practical lab techniques together. | | | | | | |
| CO3. | Apply the spectroscopic techniques for the determination of molecular structures of organic molecules. | | | | | | |
| CO4. | Present their work with practical skills and the awareness of health and safety procedures. | | | | | | |
| | PSO1 | PSO2 | PSO3 | PSO4 | PSO5 | PSO6 | PSO7 |
| CO1 | 1 | 3 | 5 | 3 | 5 | 5 | 2 |
| CO2 | 2 | 3 | 5 | 3 | 3 | 4 | 3 |
| CO3 | 1 | 3 | 5 | 2 | 3 | 3 | 2 |
| CO4 | 4 | 3 | 3 | 4 | 5 | 3 | 3 |

SEMESTER-II

| I.K. GUJRAL PUNJAB TECHNICAL UNIVERSITY DEPARTMENT OF CHEMICAL SCIENCES | | | | |
|--|--|------------|------------|------------------|
| Course Name | M.Sc. Chemistry | | | |
| Subject Code: | CHL411-18 | | | |
| Subject Title: | INORGANIC CHEMISTRY-II | | | |
| Contact Hours: | L:4 | T:0 | P:0 | Credits:4 |
| Examination Duration (hours) | 3 | | | |
| Objective(s): | To impart concepts in organometallic chemistry and structural aspects of inorganic chains, rings, cages and clusters, inorganic reaction mechanism and nuclear chemistry | | | |

Details of the Course

| Unit | Contents | Contact Hours |
|-------------|--|----------------------|
| I | Organometallic Chemistry: 18 electron rule, Exceptions to eighteen electron rule, Synthesis, structure, bonding and reactivity of transition metal complexes with olefins, Cyclobutadiene Cyclopentadienyl, Cyclopentadiene, Benzenoid (metallocenes), π -allyl and Enyl System, Dynamic equilibria in allyl complexes, Differences between unconjugated & conjugated olefin ligands. Transition metal-carbon bond: Metal-alkyls (Organomercury and Grignard reagent), metal-carbenes (chromium complexes) and metal-carbides (Tungsten carbide). | 12 |
| II | Inorganic Reaction Mechanism: Lability and inertness of metal complexes, Factors effecting reaction rate, Substitution reactions in octahedral complexes, types of intermediate formed in substitution reactions, Details of mechanism of hydrolysis (under acidic and basic condition) and the stereochemistry of intermediate formed, Trans effect and their theories, oxidation-reduction reactions, Outer sphere and inner sphere reactions. Mechanism of electron transfer reaction. | 13 |
| III | Chains, Rings and Cages: Catenation, Heterocatenation, Isopolyanions, Heteropolyanions, Preparation, structure and | 10 |

| | | |
|----|--|----|
| | properties of Boranes, Diboranes, Carboranes, Borazenes, metallocene-carboranes. Metal clusters: Geometric and electronic structure, three, four and higher connect clusters, closo-, nido-, arachno-borane structural paradigm, Wade rules, Metal carbonyl cluster, heteronuclear cluster, capping rules, isolobal relationships, Zintl ions. | |
| IV | Nuclear Chemistry: Nuclear particles, forces, size, nuclear binding energy; Detection and measurement of radioactivity (G.M. Counter method); Decay kinetics-first order rate equation for radioactive disintegration; Theory of Radioactive disintegration; Radioactive series- Uranium; magic number concept; uses of radioactive and non-radioactive isotopes; transmutation of elements; purity and strength of radio isotopes, Basic principles and types of nuclear reactors; atomic energy and Q values. | 10 |

Reference Books

| S.No. | Author(s) | Title of the Book | Publisher/Year |
|-------|---|--|--|
| 1 | J.E. Huheey, Ellen A. Keiter, Richard L. Keiter | Inorganic Chemistry Principles of Structure and Reactivity, Fourth edition | Harper Collins College Publishers |
| 2 | Cotton, Wilkinson Murillo and Bochmann | Advanced Inorganic Chemistry, Sixth edition | Wiley |
| 3 | J.D. Lee | Concise Inorganic Chemistry, Fifth edition | Oxford |
| 4 | Duward Shriver, Peter Atkins, W. H. Freeman | Inorganic Chemistry, 3rd edition | W. H. Freeman and Company, New York |
| 5 | R.S. Drago | Physical Methods in inorganic Chemistry, 2nd Edition, | Affiliated East-West Press (Section 1 & 2), Reinhold New York (1968) |
| 6 | H.B. Gray | Electrons and Chemical Bonding | (Section 2), W.A. Benjamin, London (1965) |
| 7 | A.B.P. Lever | Inorganic Electronic-Spectroscopy, 2 nd Edition | Amsterdam, The Netherlands: Elsevier, 1984 |
| 8 | N.N. Greenwood and A. Earnshaw | Chemistry of Elements | Earnshaw, Pergamon Press, (Section 7) (1984) |

Course Outcomes and Mapping

| | |
|---|---|
| At the end of the course, the student will be able to | |
| CO1. | Understand the method of synthesis, bonding and reactivity of organometallic compounds. |
| CO2. | Learn the factors responsible for the stability of organometallic compounds and clusters. |
| CO3. | Understand the structures and properties of various types of inorganic chain, rings and cages. |
| CO4. | Knowledge of various reaction mechanisms (substitution reactions or electron transfer reactions) in inorganic complexes |

| CO5. Understand the basics of nuclear chemistry and radio analytical techniques. | | | | | | | |
|---|------|------|------|------|------|------|------|
| | PSO1 | PSO2 | PSO3 | PSO4 | PSO5 | PSO6 | PSO7 |
| CO1 | 1 | 1 | 4 | 1 | 5 | 3 | - |
| CO2 | 1 | - | 4 | 1 | 5 | 3 | - |
| CO3 | 1 | 1 | 4 | 1 | 4 | 3 | - |
| CO4 | 1 | - | 3 | 1 | 4 | 1 | - |
| CO5 | 1 | 4 | 2 | 1 | 1 | 3 | 1 |

| I.K. GUJRAL PUNJAB TECHNICAL UNIVERSITY | |
|--|---|
| DEPARTMENT OF CHEMICAL SCIENCES | |
| Course Name | M.Sc. Chemistry |
| Subject Code: | CHL412-18 |
| Subject Title: | REACTIVE INTERMEDIATES-II |
| Contact Hours: | L:4 T:0 P:0 Credits:4 |
| Examination Duration (hours) | 3 |
| Objective(s): | 1. To study the reaction mechanisms in various types of addition reactions, redox reactions and rearrangement reactions. 2. To predict and account for the most commonly encountered reaction mechanisms in organic chemistry. |

Details of the Course

| Unit | Contents | Contact Hours |
|-------------|---|----------------------|
| I | Addition to carbon-carbon and carbon-hetero multiple bonds: Mechanistic and stereochemical outcome in the addition of electrophile, nucleophile, free radicals, Hydration of olefins and acetylenes, addition of halogens, Electrophilic additions involving metal ions, oxymercuration, hydroxylation, Michael addition, Sharpless asymmetric epoxidation. Free-Radical addition of hydrogen halides, halomethanes, thiols <i>etc.</i> to carbon-carbon multiple bonds Hydration and addition of alcohols to aldehydes and ketones. Addition of nucleophilic carbon to carbonyl groups: Grignard reagents, organozinc, organolithium and Gillman reagents to carbonyl and unsaturated carbonyl compounds. Carbenes and their additions to double bonds, Simmon-Smith reaction, Mannich, Stobbe, Darzen, Wittig, Wittig-Horner and Benzoin reactions. | 12 |
| II | Oxidation reactions: Introduction, different oxidative processes, Mechanistic study of the oxidation reactions. Oxidation of hydrocarbons: oxidation of methylene, oxidation of aryl methanes, allylic oxidation of olefins, dehydrogenation by quinones, SeO ₂ | 12 |

| | | |
|-----|--|----|
| | and Pb(OAc) ₄ , Formation of C-C bond in phenol coupling-acetylene coupling-allylic oxidation. Oxidation of alcohols: Swern Oxidations, PCC, PDC oxidation, oxidation using different metal based and non-metal based reagents, oxidation of glycols, halides and amines to aldehydes and ketones, ozonolysis-oxidation of olefinic double bonds, oxidation of α,β -unsaturated carbonyl compounds, ketones, Baeyer-Villiger oxidation. | |
| III | Reduction reactions: Introduction. Different reductive processes, Catalytic hydrogenation: selectivity, hydrogenation of alkenes and its stereochemical and mechanistic aspects, hydrogenation of alkynes, aromatic compounds, carbonyl compounds–aldehydes, ketones, acids, ester and nitriles, epoxides, nitro, nitroso, azo and oxime groups. homogenous hydrogenation, reduction by dissolving metals: reduction of carbonyl compounds, conjugated systems, alkynes, aromatic compounds, clemmensen reduction. Reduction by hydride transfer reagents: Lithium aluminium hydride, alkoxy substituted LAH, diisobutyl aluminium hydride, Sodium borohydride, Sodium cyanoborohydride, Sodium triacetoxyborohydride, tin hydride, trialkyl tin hydride, trialkyl silanes, diborane, diisopentyl borane, hexyl borane, 9-BBN, isopinocampheyl and diisopinocampheyl borane. Wolf-Kishner reduction. | 12 |
| IV | Rearrangements: General mechanistic consideration: Types of migration, Rearrangements on deficient carbons: Wagner-Meerwein rearrangement, Pinacol-pinacolone, Favorskii rearrangement, Allylic rearrangement, Isonitrile-Nitrile rearrangement. Rearrangements on carbonyl group: Benzil-Benzilic acid rearrangement. Rearrangements on heteroatoms: Hofmann rearrangement, Beckmann, Schmidt, Baeyer-Villiger, Criegee rearrangement. Rearrangements in pericyclic reactions: Cope rearrangement, Claisen rearrangement. Other rearrangements: Demjanov, Arndt-Eistert synthesis, Neber, Curtius, Shapiro reaction, Fries rearrangement, dienone-phenol, Wolf, Stevens (in cyclic systems). | 9 |

Reference Books

| S.No. | Author(s) | Title of the Book | Publisher |
|-------|--|--|---|
| 1 | W. Carruthers and I. Coldham | Some Modern Methods of Organic Synthesis, IV Edition | Cambridge University Press, 2004 |
| 2 | Francis A. Carey and Richard J. Sundberg | Advanced Organic Chemistry Vol. A and Vol. B, fourth Edition | Kluwer Academic publishers, New York 2002 |
| 3 | Jerry March | Organic Reaction Mechanism | John Wiley Ed. 5, 2002 |
| 4 | John McMurry and Eric Simanek | Fundamentals of Organic Chemistry | Cengage Learnings |
| 5 | R.O.C. Norman | Principles of organic synthesis | Chapman and Hall, London. 1980 |

| | | | |
|---|------------------------------|-------------------------------|--|
| 6 | T.L. Gilchrist and C.W. Rees | Carbenes, Nitrenes and Arynes | Thomas Nelson and Sons Ltd., London |
| 7 | H.O. House | Modern Synthetic Reactions | The Benjamin Cummings Publishing Company, London, 1972 |

Course Outcomes and Mapping

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

- CO1.** predict and account for the most commonly encountered reaction mechanisms in organic chemistry
- CO2.** predict the relationships between organic chemical structures and their reactivity.
- CO3.** learn the fundamental and advanced concepts in reaction mechanisms in organic chemistry along with the study of reaction mechanisms in various types of addition, redox and rearrangement reactions.
- CO4.** study the new methodologies for altering the reactivity patterns of reactive intermediates.
- CO5.** synthesize various molecules using combinations of reactive intermediates.

| | PSO1 | PSO2 | PSO3 | PSO4 | PSO5 | PSO6 | PSO7 |
|-----|------|------|------|------|------|------|------|
| CO1 | 1 | 3 | 4 | 1 | 1 | 3 | 2 |
| CO2 | 1 | 3 | 4 | 1 | 3 | 3 | 3 |
| CO3 | 2 | 3 | 4 | 1 | 1 | 3 | 3 |
| CO4 | 1 | 4 | 4 | 1 | 2 | 5 | 2 |
| CO5 | 1 | 4 | 4 | 1 | 3 | 5 | 2 |

| I.K. GUJRAL PUNJAB TECHNICAL UNIVERSITY DEPARTMENT OF CHEMICAL SCIENCES | | | | |
|--|---|------------|------------|------------------|
| Course Name | M.Sc. Chemistry | | | |
| Subject Code: | CHL413-18 | | | |
| Subject Title: | PHYSICAL CHEMISTRY-II | | | |
| Contact Hours: | L:4 | T:0 | P:0 | Credits:4 |
| Examination Duration (hours) | 3 | | | |
| Objective(s): | To impart students knowledge regarding basics of Quantum mechanics and their applications for solving various problems in physical chemistry. | | | |

Details of the Course

| Unit | Contents | Contact Hours |
|------|--|---------------|
| I | An introduction to quantum mechanics; quantum mechanics vs. classical mechanics, wave–particle duality, and uncertainty principle. Postulates of Quantum mechanics, Operators and observables, Hermitian operators, Normality and orthogonality of functions. Wave function and interpretation; time-dependent and time-independent Schrödinger equation, Problems related to eigen value. Solution of Schrodinger equation for particle in one and three dimensional box. | 13 |
| II | Application of Schrodinger wave equation to Harmonic oscillator and Rigid rotor; orbital and spin angular momentum; ordinary angular momentum; Eigen functions and Eigen values of angular momentum; ladder operator; addition of angular momenta; spin and antisymmetry; and Pauli exclusion principle. | 10 |
| III | Outline of various steps in the solution of the electronic Schrödinger equation for hydrogen atom; Radial and angular parts of the hydrogenic wave functions (atomic orbitals) and their variations for 1s, 2s, 2p, 3s, 3p and 3d orbitals; Significance of Quantum numbers; Need for approximation methods; Perturbation theory; variation theorem; linear variation principle; and application of variation method and perturbation to helium. | 12 |
| IV | Electronic configuration; Russel-Saunders terms and coupling schemes; Slater-Condon parameters; Term separation energies of the | 10 |

| | | |
|--|--|--|
| | p ⁿ and d ⁿ configurations; magnetic effects like spin orbit coupling and Zeeman splitting; and introduction to methods of self-consistent virial theorem. Huckel theory of conjugates systems; application to ethylene and butadiene; bond order and charge density calculations. | |
|--|--|--|

Reference Books

| S.No. | Author(s) | Title of the Book | Publisher/Year |
|-------|-------------------------------|--|--------------------------------|
| 1 | I.N. Levine | Quantum Chemistry, 5 th edition | Prentice Hall (2006) |
| 2 | F.L. Pilar | Elementary Quantum Chemistry | McGraw Hill (1968) |
| 3 | N.H. March | Self-Consistent Fields in Atoms | Pergamon Press (1975) |
| 4 | A.K. Chandra | Introductory Quantum Chemistry | Tata-McGraw Hill (1988) |
| 5 | P.W. Atkins and R.S. Friedman | Molecular Quantum Mechanics, 4 th edition | Oxford University Press (2004) |

Course Outcomes and Mapping

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

- CO1.** Understand the need for quantum mechanical formalism and basic principles.
- CO2.** Appreciate the importance and implication of generalized uncertainty principle in quantum mechanics.
- CO3.** Solve the eigen value problems.
- CO4.** Have a better understanding of the mathematical foundations of angular momentum of microscopic particles.
- CO5.** Apply Schrodinger wave equation and approximation methods for problem solving in quantum mechanics.
- CO6.** Rationalise the concept of bonding in conjugated polyenes.

| | PSO1 | PSO2 | PSO3 | PSO4 | PSO5 | PSO6 | PSO7 |
|-----|------|------|------|------|------|------|------|
| CO1 | 1 | 4 | 4 | 2 | ... | 2 | 4 |
| CO2 | 1 | 2 | 4 | 2 | ... | 2 | 4 |
| CO3 | 2 | 5 | 3 | ... | ... | 3 | 4 |
| CO4 | 1 | 5 | 3 | 2 | 1 | 3 | 4 |
| CO5 | ... | 5 | 3 | ... | 2 | 3 | 4 |
| CO6 | ... | 4 | 3 | 2 | 1 | 2 | 3 |

| I.K. GUJRAL PUNJAB TECHNICAL UNIVERSITY DEPARTMENT OF CHEMICAL SCIENCES | | | | |
|--|---|------------|------------|------------------|
| Course Name | M.Sc. Chemistry | | | |
| Subject Code: | CHL414-18 | | | |
| Subject Title: | SPECTROSCOPY-II | | | |
| Contact Hours: | L:4 | T:0 | P:0 | Credits:4 |
| Examination Duration (hours) | 3 | | | |
| Objective(s): | To provide knowledge of advanced spectroscopic techniques for identification and elucidation of structures of molecules | | | |

Details of the Course

| Unit | Contents | Contact Hours |
|------|--|---------------|
| I | <p>Microwave spectroscopy: Rigid and non-rigid rotator, Intensities of spectral lines, isotopic substitution effects, polyatomic linear and symmetric top molecules, Stark effect</p> <p>Vibrational Spectroscopy: Types of vibrations, overtones, combination and difference bands, Fermi resonance, group vibrations, Harmonic and anharmonic oscillators, absorptions of radiation by molecular vibrations, selection rules, force constant, frequency of vibrational transitions of HCl, vibrations in a polyatomic molecule, 3N-6 and 3N-5 rules, Applications</p> | 12 |
| II | <p>Raman Spectroscopy: Introduction, vibrational-rotational Raman Spectra, selection rules, mutual exclusion principle, anisotropic polarizability, Stokes, anti-Stokes lines, vibrational Raman spectra of CO₂ and H₂O, polarised and depolarised Raman Lines.</p> <p>Mössbauer Spectroscopy: Basic principles, Spectral parameters and display, simple spin states ($I = 1/2, 3/2$), higher spin states ($I > 3/2$), magnetic splitting, quadruple splitting, additive model application to ⁵⁷Fe, ¹¹⁹Sn</p> | 10 |
| III | <p>Nuclear Quadruple Resonance Spectroscopy: Introduction, experimental considerations, fundamentals of NQR spectroscopy, origin of EFG, measurement of energy differences between two nuclear spin states, the asymmetry parameter, effects of the magnetic field, interpretation of the spectra, application of NQR spectroscopy</p> <p>Photoelectron Spectroscopy-I: Introduction, photoelectron spectroscopy, chemical shift, X-ray photoelectron spectroscopy,</p> | 11 |

| | | |
|----|---|----|
| | molecular orbital diagrams of nitrogen and oxygen and their XPS spectra-ESCA. | |
| IV | Photoelectron Spectroscopy-II: Ultraviolet photoelectron spectroscopy (UPS), PES spectrum of nitrogen sample, vibrational structure in the N ₂ UPS spectrum, chemical shifts in XPS, exchange splitting and shake up process. Electron Paramagnetic Resonance Spectroscopy: Principle, Spectral display, hyperfine splitting in isotropic systems involving more than one nucleus, Factors affecting magnitude of g values, zero field splitting and Kramer's degeneracy, Spectrum of benzene radical anion, methyl radical, CH ₂ OH, cyclopentadienyl, cycloheptatrienyl radical, pyrazine anion, pyrazine anion, Spectra of triplet states. | 12 |

Reference Books

| S.No. | Author(s) | Title of the Book | Publisher/Year |
|-------|---|---|---|
| 1 | R.S. Drago | Physical Methods in inorganic Chemistry | Affiliated East-West Press (Section 1& 2) 2nd Edition, Reinhold New York (1968) |
| 2 | C. N. Banwell | Fundamentals of Molecular Spectroscopy | McGraw-Hill, 1966 |
| 3 | R. V. Parish | NMR, NQR, EPR & Mossbauer spectroscopy in Inorganic Chemistry | Ellis Horwood, London, 1990 |
| 4 | G. M. Barrow | Introduction to Molecular Spectroscopy | McGraw-Hill |
| 5 | E. A. Ebsworth, S.Craddock and D.W. H. Rankin | Structural methods in Inorganic Chemistry | Blackwell Scientific Publications (1991) |
| 6 | C.N.R. Rao and J.R. Ferraro | Spectroscopy in Organic Chemistry | Vol. I, Academic Press, 1971 |

Course Outcomes and Mapping

| | | | | | | | |
|---|---|------|------|------|------|------|------|
| At the end of the course, the student will be able to | | | | | | | |
| CO1. | Learn the fundamental and advanced concepts of Microwave, Infrared-Vibration-rotation Raman and infra-red Spectroscopy and their applications for chemical analysis | | | | | | |
| CO2. | Understand Electronic spectroscopy of different elements and simple molecules. | | | | | | |
| CO3. | Study the concepts and principles of Mössbauer Spectroscopy and its application. | | | | | | |
| CO4. | Apply Nuclear Quadruple Resonance and Electron Spin Resonance Spectroscopy for organic compounds analysis. | | | | | | |
| CO5. | Solve structural problems based on these techniques. | | | | | | |
| | PSO1 | PSO2 | PSO3 | PSO4 | PSO5 | PSO6 | PSO7 |
| CO1 | 3 | 3 | 3 | 1 | 3 | 3 | 3 |
| CO2 | 3 | 4 | 3 | 1 | 3 | 3 | 3 |

| | | | | | | | |
|-----|---|---|---|---|---|---|---|
| CO3 | 3 | 4 | 2 | - | 3 | 4 | 3 |
| CO4 | 3 | 3 | 2 | - | 3 | 4 | 4 |
| CO5 | 3 | 5 | 2 | 2 | 4 | 4 | 3 |

| I.K. GUJRAL PUNJAB TECHNICAL UNIVERSITY DEPARTMENT OF CHEMICAL SCIENCES | | | | |
|--|--|------------|------------|------------------|
| Course Name | M.Sc. Chemistry | | | |
| Subject Code: | CHL415A-18 | | | |
| Subject Title: | CHEMISTRY OF MATERIALS | | | |
| Contact Hours: | L:4 | T:0 | P:0 | Credits:4 |
| Examination Duration (hours) | 3 | | | |
| Objective(s): | To introduce the students in the area of liquid crystalline materials and solid state material chemistry and also to impart fundamental and advance understanding on nanoscale materials, their properties and applications. | | | |

Details of the Course

| Unit | Contents | Contact Hours |
|------|--|---------------|
| I | Interfaces and Liquid Assemblies: Order in liquids, Surfactants, Micelles, Vesicles and biological membranes, Surface self-assembled monolayers, Liquid crystals, Nature and structure, Design of liquid crystalline materials, Supramolecular liquid crystals, Liquid crystal displays, Inorganic liquid crystals | 11 |
| II | Solid-State and Materials Chemistry: Synthesis of material, The formation of bulk material, Chemical deposition, Metal oxides: Monoxides of the 3d metals, higher oxides and complex oxides: Spinel molecule, Inverse and normal, Perovskites and related phase, High temperature superconductor, Thermochromics and photochromic materials, Oxide glasses, Aluminophosphates, Silicates. Zeolites, Structure and composition, Synthesis, MFI Zeolites in petroleum industry, Layered Solids and Intercalates: Characteristics, Graphite Intercalates, Coordination Polymers: Introduction, Metal Organic Frameworks, Guest properties of metal organic framework, applications of coordination polymers | 12 |
| III | Inorganic pigments: Coloured solids, White and black pigments, Semiconductors: Group 14 semiconductors, Semiconductor system isoelectronic with Silicon. Material used in Light emitting diodes, Defects in crystals, Color Centers, Quantum dots. | 10 |
| IV | Nanochemistry and Nanomaterials: Nanotechnology: The 'Top Down' and 'Bottom Up' Approaches, Template synthesis using frameworks, supports and substrates, Microfabrication, Nanofabrication and Soft Lithography Nanoparticles: | 12 |

| | | |
|--|---|--|
| | Nanoparticles and Colloids, Gold Nanoparticles, Non-Spherical Nanoparticle, Endohedral Fullerenes, Nanotubes and Graphene | |
|--|---|--|

Reference Books

| S.No. | Author(s) | Title of the Book | Publisher/Year |
|-------|--|---|--------------------------------|
| 1 | P. Oswald, P. Pieranski | Nematic and Cholesteric liquid crystals | Taylor and Francis Group, 2005 |
| 2 | Atkins, Overton, Rourke, Weller, Armstrong | Inorganic chemistry | Fifth edition, 2010, oxford |
| 3 | J. W. steed, J. L. Atwood | Supramolecular Chemistry | second edition 2009, Wiley |

Course Outcomes and Mapping

| | | | | | | | |
|--|------|------|------|------|------|------|------|
| At the end of the course, the student will be able to | | | | | | | |
| CO1. Understand the basic concepts and formation of various supramolecular assemblies. CO2. Know the types and structure of liquid crystals and their applications. CO3. Learn the common and important synthesis methods, structure and composition of solid state materials and their applications in industries. CO4. Understand the concepts, mechanism and applications of inorganic pigments. CO5. Learn the various approaches for the synthesis of nanoscale materials/nanoparticles and their properties and applications. | | | | | | | |
| | PSO1 | PSO2 | PSO3 | PSO4 | PSO5 | PSO6 | PSO7 |
| CO1 | 2 | 2 | 4 | 2 | 2 | 2 | 2 |
| CO2 | 1 | 3 | 4 | 2 | 3 | 3 | 4 |
| CO3 | 4 | 3 | 5 | 4 | 3 | 4 | 4 |
| CO4 | 1 | 3 | 4 | 2 | 2 | 3 | 2 |
| CO5 | 3 | 3 | 4 | 4 | 3 | 5 | 4 |

| I.K. GUJRAL PUNJAB TECHNICAL UNIVERSITY DEPARTMENT OF CHEMICAL SCIENCES | | | | |
|--|---|------------|------------|------------------|
| Course Name | M.Sc. Chemistry | | | |
| Subject Code: | CHL415B-18 | | | |
| Subject Title: | CHEMICAL BIOLOGY | | | |
| Contact Hours: | L:3 | T:0 | P:0 | Credits:3 |
| Examination Duration (hours) | 3 | | | |
| Objective(s): | Chemical Biology is one of the emerging interdisciplinary branch of chemistry which helps in exploring and understanding the various biological phenomena occurring at molecular level. This involves application of principles of physical, inorganic, organic and analytical chemistry to investigate the molecular properties of various macromolecular assemblies to understand the cellular behaviour. Therefore the objective of teaching this subject of Chemical Biology is to prepare the students who are interested in having their careers in Bioengineering, Pharmacology, Molecular Medicine, Biochemistry and Molecular Biology and they can have an opening in these areas. | | | |

Details of the Course

| Unit | Contents | Contact Hours |
|-------------|---|----------------------|
| I | Fundamentals of Chemical Biology : General Introduction to Chemical Biology, Central Dogma of Molecular Biology, Molecular Biology as a tool of Chemical Biology, Genes, Genomes, Biooligomers, DNA libraries, protein libraries, Combinatorial synthesis of biomolecules. | 8 |
| II | Molecular Selection & Evolution: Chemical Biology & Origin of Life, Natural selection, Evolution of Protein functions & nucleic acids, Catalytic antibodies. Structure of Biomolecules: General Introduction to biological macromolecules, Structure of Proteins, Carbohydrates, Nucleic acids, lipids & lipid assemblies, Structural forces in biological macromolecules. | 5 8 |
| III | Chemical & Biological synthesis of Biomolecules: General Introduction to synthesis in Chemical Biology, Chemical synthesis of peptides, proteins, oligosaccharides, lipids and nucleic acids, Biological synthesis of lipids, nucleic acids and proteins. | 12 |
| IV | Molecular Recognition & Binding: Molecular recognition & binding in Chemical Biology, Analysing Molecular Recognition & binding, Biological Molecular recognition studies. | 6 |

| | | |
|--|---|---|
| | Application of various techniques in studying biomolecules: Mass Spectrometry, NMR, Electronic & vibrational spectroscopy, Electrophoresis, X-Ray Diffraction | 6 |
|--|---|---|

Reference Books

| S.No. | Author(s) | Title of the Book | Publisher/Year |
|-------|-----------------------------------|---|------------------------------------|
| 1. | Andrew Miller & Julian Tanner | Essentials of Chemical Biology: Structural & Dynamics of Biomolecules | John Wiley & Sons, USA. 2008 |
| 2. | David Van Vranken & Gregory Weiss | Introduction to Bioorganic Chemistry & Chemical Biology | Taylor & Francis Group. 2013 |
| 3. | D. L. Nelson & M.M. Cox | Lehninger Principles of Biochemistry | WH Freeman Company, New York. 2008 |

Course Outcomes & Mapping

| | | | | | | | |
|---|---|------|------|------|------|------|------|
| At the end of the course, the student will be able to | | | | | | | |
| CO1. | Understand the chemical principles that govern structure & functioning of biomolecules such as Proteins, Carbohydrates, Lipids and Nucleic acids etc. | | | | | | |
| CO2. | Learn chemical synthesis of various Biomolecules. | | | | | | |
| CO3. | Acknowledge the role of Chemical Biology in kinetics of molecular recognition of functional & structural biomolecules. | | | | | | |
| CO4. | Explore new frontiers of research in biology using chemical methods. | | | | | | |
| CO5. | Learn to apply various analytical techniques to understand functional properties of biomolecules. | | | | | | |
| | PSO1 | PSO2 | PSO3 | PSO4 | PSO5 | PSO6 | PSO7 |
| CO1 | 2 | 4 | 3 | 3 | 4 | 5 | 4 |
| CO2 | 2 | 3 | 3 | 4 | 4 | 5 | 4 |
| CO3 | - | 4 | 3 | 3 | 4 | 5 | 4 |
| CO4 | 2 | 3 | 3 | 3 | 4 | 5 | 4 |
| CO5 | 2 | 5 | 3 | 3 | 4 | 5 | 4 |

| I.K. GUJRAL PUNJAB TECHNICAL UNIVERSITY | | | | |
|--|--|------------|------------|------------------|
| DEPARTMENT OF CHEMICAL SCIENCES | | | | |
| Course Name | M.Sc. Chemistry | | | |
| Subject Code: | CHP416-18 | | | |
| Subject Title: | PHYSICAL CHEMISTRY LAB | | | |
| Contact Hours: | L:0 | T:0 | P:6 | Credits:3 |
| Examination Hours: | 6 | | | |
| Objective(s): | To provide students practical knowledge and skills about various topics taught in theory class of physical chemistry | | | |

Details of the Course

Any fifteen experiments to be performed out of the following:

1. Find graphically the equivalent conductance at infinite dilution of weak electrolyte and hence determine the thermodynamic dissociation constant of the weak acid.
2. Determine the equivalent conductance of a strong electrolyte at several concentrations and verify the Onsager's equation.
3. Determine the equivalent conductance of a weak electrolyte at infinite dilution using Kohlraush law.
4. To determine relative strength of two acids by conductance measurements.
5. Determine the solubility of a sparingly soluble salt in water using conductance measurements.
6. Determine the end point of some typical titrations by conductometric method.
7. Determine the composition of a mixture of acetic acid and hydrochloric acid by conductometric titration.
8. Study the kinetics of saponification of ethyl acetate by sodium hydroxide and hence determine the activation energy of the reaction.
9. Investigate the reaction between acetone and iodine.
10. Determine the relative strength of two acids studying the hydrolysis of an ester.
11. Study the kinetics of decomposition of the complex formed between sodium sulphide and sodium nitroprusside spectrophotometrically and find the rate constant and order of the reaction.
12. Investigate the inversion of cane sugar in presence of an acid.
13. Obtain a calibration curve for a given compound and verify Beer-Lambert law.
14. Study the complex formation between Fe (III) and salicylic acid, and find the formula and the stability of the complex.
15. Determine the concentration of Nickel in solution by spectrophotometric titration.
16. Determination of specific and molar refraction of a liquid by Abbe refractometer.
17. Determine the refraction equivalents of C, H, and Cl atoms.
18. Determine the composition of mixture of two liquids by refractive index measurements.

19. Determination of surface tension of given liquid by a) drop number method and b) drop weight method using stalagmometer.
20. Determine the critical micellar concentration of soap (sodium or potassium lauryl sulphate) by surface tension measurements.
21. Determine the parachor of the mixture using surface tension measurements.
22. Compare the cleansing power of two samples of detergent.
23. Determination of transition temperature of given substance by thermometric or dilatometric method.
24. Find water equivalent and heat of neutralization of strong acid vs strong base, weak base vs. strong acid using Dewar's flask.

Reference Books

1. Advanced Practical Physical Chemistry by J.B. Yadav.
2. Findlay's Practical Physical Chemistry.

Course Outcomes and Mapping

At the end of the course, the students will be able to

- CO1.** Understand the basic procedures for carrying out a physical chemistry practical like preparation and standardisation of solutions, handling the equipments and measuring with precision.
- CO2.** Correlate the theoretical and practical aspects and know about the limits of the experimental error.
- CO3.** Determine the various physical parameters for the various problems under study which in turn will enhance their problem solving and analytical skills.
- CO4.** Verify various laws studied in the theory part.

| | PSO1 | PSO2 | PSO3 | PSO4 | PSO5 | PSO6 | PSO7 |
|-----|------|------|------|------|------|------|------|
| CO1 | 1 | 5 | 5 | 3 | 5 | 5 | 3 |
| CO2 | 2 | 4 | 5 | 3 | 5 | 2 | 4 |
| CO3 | 2 | 5 | 5 | 2 | 4 | 3 | 5 |
| CO4 | 2 | 5 | 5 | 1 | 4 | 2 | 5 |

| I.K. GUJRAL PUNJAB TECHNICAL UNIVERSITY DEPARTMENT OF CHEMICAL SCIENCES | | | | |
|--|---|------------|------------|------------------|
| Course Name | M.Sc. Chemistry | | | |
| Subject Code: | CHP417-18 | | | |
| Subject Title: | ADVANCED CHEMISTRY LAB-I | | | |
| Contact Hours: | L:0 | T:0 | P:6 | Credits:3 |
| Examination Hours: | 6 | | | |
| Objective(s): | To provide illustrative experiments to support the material taught in the theory courses and to give the students practical experience in techniques used in the synthesis, isolation, characterization and structure determination of inorganic compounds. | | | |

Details of the Course

| S.No. | Contents |
|--------------|---|
| I | Inorganic Practicals <ol style="list-style-type: none"> 1. Preparation of Octahedral and Tetrahedral Complexes of dichlorodipyridylcobalt(II), Differentiate them using IR, UV and Magnetic Properties. Estimate Co(II) from one of them. 2. Preparation of cis-and trans-potassium Dioxalato Diaquochromate (III). Interpretation of IR, UV and Magnetic Properties. Estimation of Chromium. 3. Preparation of Salicylamide complexes of Copper(II). IR, UV, magnetic data and analysis of Cu(II). 4. To separate the mixture of metal ions (Cr^{3+}, Ni^{+2}, Cu^{+2}, Zn^{+2}, Fe^{+2}) using thin layer and column chromatography. 5. To perform the solvent extraction for the recovery of metal ions (Cr^{3+}, Ni^{+2}, Cu^{+2}, Zn^{+2}, Fe^{+2}) from aqueous medium. |
| II | Organic Practicals <ol style="list-style-type: none"> 1. Synthesize (a) 2,4-dinitro-1-chlorobenzene from chlorobenzene, (b) mixture of <i>o</i>- and <i>p</i>-nitrophenols from phenol and (c) <i>p</i>-nitroacetanilide from acetanilide and make comparison of the reactivity of various substrates and reaction conditions used for performing nitration in each experiment. (Book 2, pp 978-979, 919-20) 2. Synthesis of benzalacetophenone by condensation of benzaldehyde with acetophenone and study its bromination and subsequent de-bromination. (Book 1, pp 242-247, Book 3 pp 361-365) |

| | |
|--|---|
| | 3. Synthesis of 2-chloro-4-bromo-6-iodoaniline from aniline. (Book 1, pp 292-299). 4. The epoxidation of benzalacetophenone to its epoxide and study its reactivity towards hydroxyl ion. (Book 3, pp 363-364). 5. Michael addition of aniline to benzalacetophenone. (Book 1, p 247). 6. Conversion of benzalacetophenone to its oxime and its transformation to amide and oxazole derivatives. (Book 1, pp 242-247, Book 3 pp 361-365) |
|--|---|

Reference Books

| S.No. | Author(s) | Title of the Book | Publisher |
|-------|--|--|--|
| 1 | R.M. Roberts, Gilbert, L. B. Rodewald and A.S. Wingrove. Holt, | An Introduction to Modern Experimental Organic Chemistry, | Ranehart and Winston Inc., J. C New York 1969. |
| 2 | Arthur Israel Vogel (Author) | Vogel's Text Book of Practical Organic Chemistry, 5th Edition. | Longman, 1961 . |
| 3 | R. Adams, J.R. Johnson | Laboratory Experiments in Organic Chemistry | Macmillan; 7th edition (1979) |
| 4 | G. Marr and B.W. Rockett | Practical Inorganic Chemistry | |
| 5 | W.L. Jolly | The Synthesis and Characterization of Inorganic Compounds | |

Course Outcomes and Mapping

| The students will learn CO1. Preparation of different inorganic complexes. CO2. Purification and crystallisation of inorganic compounds. CO3. Interpretation of compounds using UV-Vis, FT-IR techniques. CO4. Measurement of various physical properties such as magnetic moment of complexes. CO5. Applying related experiments for their research work. | | | | | | | |
|--|------|------|------|------|------|------|------|
| | PSO1 | PSO2 | PSO3 | PSO4 | PSO5 | PSO6 | PSO7 |
| CO1 | 5 | 1 | 4 | 2 | 5 | 2 | - |
| CO2 | 5 | 1 | 4 | 1 | 5 | 2 | - |
| CO3 | 5 | 4 | 5 | - | 5 | 3 | 4 |
| CO4 | 3 | 4 | 5 | - | 4 | 2 | 2 |
| CO5 | 5 | 2 | 2 | - | 5 | 1 | - |

SEMESTER-III

| I.K. GUJRAL PUNJAB TECHNICAL UNIVERSITY | | | | |
|--|---|------------|------------|------------------|
| DEPARTMENT OF CHEMICAL SCIENCES | | | | |
| Course Name | M.Sc. Chemistry | | | |
| Subject Code: | CHL501-18 | | | |
| Subject Title: | INORGANIC CHEMISTRY-III | | | |
| Contact Hours: | L:4 | T:0 | P:0 | Credits:4 |
| Examination Duration (hours) | 3 | | | |
| Objective(s): | To provide basic concepts of group theory and the inorganic biochemistry and catalysis. | | | |

Details of the Course

| Unit | Contents | Contact Hours |
|-------------|---|----------------------|
| I | Symmetry and Group Theory: Symmetry elements, Symmetry operations, Symmetry elements of commonly occurring molecules like NH ₃ , CH ₄ , SF ₆ , PF ₅ , SF ₄ , Ni(CO) ₄ , Fe(CO) ₅ , determination of point groups, genesis and use of character table, reducible and irreducible representation determination. Solid State Chemistry: Determination of points groups; types of close packing, packing efficiency, radius ratio, polyhedral discretion of solids, structure type: NaCl, ZnS, wurtzite, rutile, perovskite, spinels. | 12 |
| II | Bio-Inorganic Chemistry: Transition elements in biology- their occurrence and function, active site structure and function of metalloproteins and metalloenzymes. O ₂ binding properties of heme and non-heme proteins, Co-operative effect, Bohr Effect, Electron transfer proteins, rubridoxin, feredoxin and cytochromes, Vitamin B ₁₂ and cytochrome P ₄₅₀ and their mechanism of action. Biological N ₂ fixation, molybdenum nitrogenase, spectroscopic and other evidence, other nitrogenases model systems. | 12 |
| III | Catalysis: Turnover number, turnover frequency, homogenous and heterogenous catalysis, (involving oxidative addition, reductive elimination, migratory insertion, hydride elimination, trans metallation, metal carbonyls hydroformylation, Olefin metathesis, cross coupling reactions, asymmetric synthesis). | 11 |
| IV | Inorganic Polymers: Types of inorganic polymers, Comparison with organic polymers, synthesis, structure aspects and application | 10 |

| | | |
|--|--|--|
| | of silicones, polyphosphazenes, Tri- and Tetra- Phosphonitrilic halides, ultraphosphate, borophosphate and chalcogenide glasses. | |
|--|--|--|

Reference Books

| S.No. | Author(s) | Title of the Book | Publisher/Year |
|-------|--|---|---|
| 1 | R.S. Drago | Physical Methods in inorganic Chemistry | Affiliated East-West Press (Section 1& 2) 2nd Edition, Reinhold New York (1968) |
| 2 | H.B. Gray | Electrons and Chemical Bonding | (Section 2), W.A. Benjamin, London (1965) |
| 3 | F.A. Cotton and G.W. Wilkinson | Advanced Inorganic Chemistry | John Wiley and Sons, 6th edition, John Wiley New York (1999) |
| 4 | J.E. Huheey | Inorganic Chemistry, Principles of Structure and Reactivity | Harper International, SI Edition, 3rd Edition, Harper London (1978) |
| 5 | G. Wilkinson (Ed.) | G. Wilkinson (Ed.) | Pergamon, Pergamon Oxford (1982) |
| 6 | N.N. Greenwood and A. Earnshaw | Chemistry of Elements | Pergamon Press, (Section 7) (1984) |
| 7 | Christopher Master | Homogenous Transition metal catalysis | (Section 8) (1981) |
| 8 | P. Atkins, T. Overton, J. Rourke, M. Weller, F. Armstrong, M. Hagerman | Inorganic Chemistry, 5 th edition | W. H. Freeman and Company, New York |

Course Outcomes and Mapping

| | | | | | | | |
|---|------|------|------|------|------|------|------|
| <p>The students will acquire knowledge of</p> <p>CO1. Concepts of symmetry and group theory in solving chemical structural problems.</p> <p>CO2. Use of character tables and projection operator techniques.</p> <p>CO3. Structure and biological functions of biomolecules and the role of metals in biology.</p> <p>CO4. Basic concepts of catalysis and reaction mechanisms using various transition metal complexes.</p> <p>CO5. Possible types, synthetic methodology and structure of inorganic polymers and their applications.</p> | | | | | | | |
| | PSO1 | PSO2 | PSO3 | PSO4 | PSO5 | PSO6 | PSO7 |
| CO1 | 2 | 3 | 4 | - | - | 2 | 2 |
| CO2 | 2 | 3 | 5 | 2 | 2 | 2 | 2 |
| CO3 | 3 | 3 | 3 | - | - | 4 | 4 |

| | | | | | | | |
|-----|---|---|---|---|---|---|---|
| CO4 | 2 | 3 | 4 | 2 | 2 | 4 | 4 |
| CO5 | 2 | 4 | 4 | - | 3 | 4 | 4 |

| I.K. GUJRAL PUNJAB TECHNICAL UNIVERSITY | | | | |
|---|--|-----|-----|-----------|
| DEPARTMENT OF CHEMICAL SCIENCES | | | | |
| Course Name | M.Sc. Chemistry | | | |
| Subject Code: | CHL502-18 | | | |
| Subject Title: | ADVANCED ORGANIC CHEMISTRY-I | | | |
| Contact Hours: | L:4 | T:0 | P:0 | Credits:4 |
| Examination Duration (hours) | 3 | | | |
| Objective(s): | To provide the comprehensive knowledge of principles of photochemistry and pericyclic reactions with learning of current applications. | | | |

Details of the Course

| Unit | Contents | Contact Hours |
|------|--|---------------|
| I. | <p>Photochemical Reactions: Interaction of electromagnetic radiation with matter, types of excitations, fate of excited molecule, quantum yield, transfer of excitation energy.</p> <p>Determination of Reaction Mechanism: Classification, rate constants and life times of reactive energy states—determination of rate constants of reactions. Effect of light intensity on the rate of photochemical reactions. Types of photochemical reactions.</p> <p>Photochemistry of Alkenes: Intramolecular reactions of the olefinic bond – geometrical isomerism, cyclization reactions, rearrangement of 1,4- and 1,5-dienes.</p> | 10 |
| II. | <p>Photochemistry of Carbonyl Compounds: Intramolecular reactions of carbonyl compounds—saturated, cyclic and acyclic, β,γ-unsaturated and α,β-unsaturated compounds, Cyclohexadienones. Intermolecular cycloaddition reactions – dimerisations and oxetane formation.</p> <p>Photochemistry of Aromatic Compounds: Isomerisation reactions, additions and substitution reactions, cyclization reactions.</p> <p>Miscellaneous Photochemical Reactions: Photo-Fries reactions of anilides, Photo-Fries rearrangement, Barton reaction. Singlet molecular oxygen reactions. Photochemical formation of smog, Photodegradation of polymers, Photochemistry of vision.</p> | 10 |
| III. | <p>Pericyclic Reactions and Molecular Orbital Symmetry: Classification of Pericyclic Reactions, Molecular Orbitals of Alkenes and Conjugated Polyene Systems, Molecular Orbitals of Conjugated Ions or Radicals, Symmetry Properties of π or σ - Molecular Orbitals, Various methods of analysis of pericyclic reactions.</p> <p>Electrocyclic Reactions: Conrotatory and Disrotatory Modes, Stereochemistry of Electrocyclic Reactions, Selection Rules for Electrocyclic Reactions, Analysis of Electrocyclic Reactions:</p> | 12 |

| | | |
|-----|---|----|
| | Correlation-Diagram approach, Perturbation Molecular Orbital (PMO) approach, Frontier Molecular Orbital (FMO) approach. Electrocyclic Reactions of Ionic Species: Three and five atom Electrocyclization reactions. | |
| IV. | <p>Cycloaddition Reactions: Stereochemical Modes of Cycloaddition, Feasibility of Cycloaddition Reactions: Orbital Symmetry Correlation-Diagram Method, Perturbation Molecular Orbital (PMO) Method, Frontier Molecular Orbital Method. [2+2] Cycloaddition reactions, [4+2] Cycloaddition reactions: Cycloaddition reactions of Diene and Dienophile, Frontier Orbital Interactions in Diels-Alder Reaction, Stereochemistry and Regiochemistry of Diels-Alder Reaction, [4+2] Cycloaddition Reactions with Allyl Cations and Allyl Anions. 1,3-dipolar cycloaddition reactions.</p> <p>Sigmatropic Rearrangements: Suprafacial and Antarafacial Processes, Analysis of [i,j] Sigmatropic Rearrangements of Hydrogen: FMO & PMO analysis, FMO & PMO Analysis of [i,j] Sigmatropic Rearrangements of Alkyl Group, [3,3] Sigmatropic rearrangements: Cope Rearrangement and Claisen Rearrangement.</p> | 13 |

Reference Books

| S.No. | Author(s) | Title of the Book | Publisher |
|-------|---|--|----------------------------------|
| 1 | John D. Coyle | Introduction to the organic photochemistry | John Wiley & Sons Ltd. |
| 2 | Dwaine O. Cowan & Ronald L. Drisko | Elements of Organic Chemistry | Plenum Press, New York |
| 3 | K.K. Rohtagi & mukerjee | Fundamentals of Photochemistry | New Age International |
| 4 | A. Gilbert, J. Baggott | Essentials of Molecular Photochemistry | CRC Press, London, UK, (1991) |
| 5 | N. J. Turro | Modern Molecular Photochemistry | University Press, Menlo Park, CA |
| 6 | Sunil Kumar, Vinod Kumar and S.P. Singh | Pericyclic Reactions | Elsevier (Academic Press) |
| 7 | Ian Fleming | Pericyclic Reactions | Oxford Science Publications |
| 8. | W. Carruthers | Cycloaddition Reactions in Organic Synthesis | Elsevier |

Course Outcomes and Mapping

| | |
|---|--|
| At the end of the course, the student will be able to | |
| CO1. | Understand the basics of photochemical reactions of alkenes, carbonyl and aromatic compounds. |
| CO2. | Understand the role of light in the organic synthetic methods and techniques for the applications in chemical reactions. |
| CO3. | Predict the concerted mechanism of the pericyclic reactions without the involvement of an intermediate. |
| CO4. | Predict the thermal or photochemical feasibility of the pericyclic reactions along with their stereo-specificity. |

| | | | | | | | |
|--|--|------------|------------|------------------|------|------|------|
| | PSO1 | PSO2 | PSO3 | PSO4 | PSO5 | PSO6 | PSO7 |
| CO1 | 1 | 3 | 4 | 3 | 2 | 4 | 2 |
| CO2 | 1 | 4 | 4 | 4 | 3 | 5 | 3 |
| CO3 | 1 | 4 | 4 | 2 | 1 | 4 | 3 |
| CO4 | 1 | 5 | 4 | 2 | 1 | 4 | 2 |
| I.K. GUJRAL PUNJAB TECHNICAL UNIVERSITY | | | | | | | |
| DEPARTMENT OF CHEMICAL SCIENCES | | | | | | | |
| Course Name | M.Sc. Chemistry | | | | | | |
| Subject Code: | CHL 503-18 | | | | | | |
| Subject Title: | PHYSICAL CHEMISTRY-III | | | | | | |
| Contact Hours: | L:4 | T:0 | P:0 | Credits:4 | | | |
| Examination Duration (hours) | 3 | | | | | | |
| Objective(s): | This course will equip students with the necessary chemical knowledge concerning the fundamentals in the basic areas of phase equilibrium, adsorption and statistical thermodynamics; with regard to various theories developed and their applicability for various systems under consideration. | | | | | | |

Details of the Course

| Unit | Contents | Contact Hours |
|-------------|---|----------------------|
| I. | Electrochemistry-II: Oxidation reduction reactions; Electrochemical cell and its types, Electrode potentials, Standard hydrogen electrode, Nernst equation, Applications of standard electrode potentials; calculation of cell potential and redox equilibrium constants, Oxidation reduction titrations. Potentiometric Methods: Reference Electrodes, Liquid Junction Potentials, Indicator electrodes, Applications. | 12 |
| II. | Solution & Phase Equilibrium Solubility and factors affecting solubility, types of solutions, ideal solution, vapour pressure of ideal solutions, boiling point diagrams of binary miscible mixtures and their distillation diagrams, azeotropes, critical solution temperatures, solubility of gases in liquids, Henry's law, Nernst distribution law, number of extractions, solutions of solids in liquids & chemical equilibrium. Gibb's phase rule, Triangular method for graphical representation of three component systems; partially miscible three liquid systems. Applications of ternary liquid diagrams; systems composed of two solids and a liquid. | 10 |
| III. | Adsorption and Surface phenomena: Surface phenomena, capillary action, pressure difference across surface (Laplace equation), vapour pressure of droplets (Kelvin equation), physical and chemical adsorption, adsorption isotherms, Derivation of Langmuir, Freundlich, Tempkin and BET absorption isotherms, Estimation of surface area by BET equation. Heterogenous catalysis, surface catalyzed unimolecular and bimolecular reactions, Retarded surface reactions, temporary and permanent catalytic poisons, activation energy for surface reactions, Numerical problems. | 10 |

| | | |
|-----|--|----|
| IV. | Statistical Thermodynamics: Thermodynamic probability and most probable distribution, Maxwell-Boltzmann distribution law; the ensemble averaging and its postulates; canonical, grand canonical, and microcanonical ensembles; Translational, rotational, vibrational, and electronic vibration function; Calculation of thermodynamic properties in terms of partition functions, Comparison of three types of statistics; Maxwell- Boltzmann, Fermi-Dirac and Bose-Einstein statistics. | 13 |
|-----|--|----|

Reference Books

| S.No. | Author(s) | Title of the Book | Publisher/Year |
|-------|--------------------------------|---|--|
| 1. | P.W. Atkins & Julio de Paula | Physical Chemistry | W H Freeman |
| 2. | G. W. Castellan | Physical Chemistry | Narosa, 4 th ed, 2004 |
| 3. | David Chandler | Introduction to Modern Statistical Mechanics | Oxford University Press |
| 4. | E. Thomas and R. Philip | Thermodynamics: Statistical Thermodynamics and Kinetics | Pearson Education, 1 st ed, 2007. |
| 5. | J.W. Moore and R.G. Pearson | Kinetics and Mechanism | John Wiley and Sons, 2 nd ed , 1981 |
| 6. | Adamson and W. Arthur | Physical Chemistry of Surfaces | Wiley-Interscience Publication, 4 th ed, 1982 |
| 7. | S.H. Maron & C.F. Prutton | Principles of Physical Chemistry, 1 st edition | Oxford and IBH (1958) |
| 8. | Skoog, West, Holler and Crouch | Fundamentals of Analytical Chemistry | Cengage Learning |

Course Outcomes and Mapping

| | | | | | | | |
|---|--|------|------|------|------|------|------|
| At the end of the course, the student will be able to | | | | | | | |
| CO1. | Solve various problems related to electrochemistry and be familiar with the various types of sensing electrodes. | | | | | | |
| CO2. | Understand and construct the phase diagrams for the ternary mixtures. | | | | | | |
| CO3. | Develop insights in the phenomenon occurring at surfaces and the theories behind them. | | | | | | |
| CO4. | Correlate classical thermodynamics with quantum mechanics by using statistical mechanical approach. | | | | | | |
| | PSO1 | PSO2 | PSO3 | PSO4 | PSO5 | PSO6 | PSO7 |
| CO1 | 1 | 5 | 5 | 3 | ... | 2 | 3 |
| CO2 | 1 | 5 | 5 | 2 | 3 | 2 | 4 |
| CO3 | 2 | 3 | 3 | 2 | 1 | 1 | 3 |
| CO4 | ... | 3 | 3 | 3 | 2 | 2 | 4 |

| I.K. GUJRAL PUNJAB TECHNICAL UNIVERSITY | | | | |
|--|--|------------|------------|------------------|
| DEPARTMENT OF CHEMICAL SCIENCES | | | | |
| Course Name | M.Sc. Chemistry | | | |
| Subject Code: | CHL504-18 | | | |
| Subject Title: | ADVANCED CHARACTERIZATION TECHNIQUES | | | |
| Contact Hours: | L:4 | T:0 | P:0 | Credits:4 |
| Examination Duration (hours) | 3 | | | |
| Objective(s): | This course will introduce the students to different techniques for characterisation of organic and inorganic materials. The emphasis will be on understanding crystal structure, morphology, microstructure, different types of phases present in a material, purity of the material. | | | |

Details of the Course

| Unit | Contents | Contact Hours |
|-------------|--|----------------------|
| I. | X-Ray diffraction: Single crystal XRD and powder XRD, Bragg's diffraction law, Unit cell, space group, element of space group, particle size analysis using Scherer formula. Thermo-Analytical Methods: Theory, instrumental requirements and methodology for thermo gravimetric analysis (TGA), differential thermal analysis (DTA) and differential scanning calorimetry (DSC), applications. | 12 |
| II. | Scanning electron microscopy: Principle, Specimen Preparation, Replicas Various-application of SEM. Transmission electron microscopy : Instrumentation, Principle, Advantage, Difference between SEM and TEM. | 10 |
| III. | Chromatographic Methods: Classification of chromatographic methods according to separation and development procedure, Stationary phase, mobile phase, retention time. Gas chromatography: Physical components, Types of column and detector, Carrier gas, Applications, Inverse Gas chromatography, GC-MS: construction and working. | 13 |
| IV. | High performance liquid chromatography: Construction and working, Partition chromatography, Normal and reverse phase chromatography, Ion exchange chromatography, Isocratic and gradient elution. Gel permeation chromatography. Electrophoresis and electrochromatography. | 10 |

Reference Books

| S.No. | Author(s) | Title of the Book | Publisher/Year |
|--------------|------------------|--------------------------|-----------------------|
|--------------|------------------|--------------------------|-----------------------|

| | | | |
|----|---|---|--------------------------------------|
| 1. | J.Goldstein, D. E. Newbury, D.C. Joy, and C.E. Lym | Scanning Electron Microscopy and X-ray Microanalysis | 2003 |
| 2. | S.L. Flegler, J.W. Heckman and K.L. Klomparens | Scanning and Transmission Electron Microscopy: A Introduction | WH Freeman & Co, 1993. |
| 3. | P.J.Goodhew, J.Humphreys, R.Beanland | Electron Microscopy and Analysis | |
| 4. | Willard, Merritt, Dean and Settle | Instrumental Methods of Analysis | CBS Publisher and Distributors.,1986 |
| 5. | W. W. Wendlandt and L. W. Collins, Dowden Hutechin and Ross | Thermal Analysis | |
| 6. | K. Tyagi, Mainak Roy, S. K. Kulshreshtha and S. Banerjee | Advanced Techniques for Materials Characterization | |

Course Outcomes and Mapping

| | | | | | | | |
|---|---|------|------|------|------|------|------|
| At the end of the course, the student will be able to | | | | | | | |
| CO1. | Understand the topography, morphology, composition, relationship between composition and material properties. | | | | | | |
| CO2. | Learn the functioning of the X-ray diffractometer, about its components and would be able to determine the crystal structure of a material, find impurity in the material, different phases present in the mixture of compound qualitative as well as functionalities | | | | | | |
| CO3. | Understand the instrumentation of TGA and also to calculate the weight loss with temperature, types of changes occurring in the material/substances during thermal breadding, enthalpy changes during heat treatment of a compound. | | | | | | |
| CO4. | Apply the knowledge of various characterization techniques in material industries, metallurgy industries, electronic industries, civil Engineering. | | | | | | |
| CO5. | Apply the quantitative and qualitative separation techniques in purification and its applications in food industry, pharmaceutical industry, purification, removal of pollutants, medicinal chemistry and essential oils. | | | | | | |
| | PSO1 | PSO2 | PSO3 | PSO4 | PSO5 | PSO6 | PSO7 |
| CO1 | 2 | 2 | 3 | ... | 3 | 3 | 3 |
| CO2 | 1 | 2 | 2 | ... | 3 | 3 | 3 |
| CO3 | 1 | 2 | 2 | 1 | 4 | 3 | 3 |
| CO4 | 2 | 1 | ... | 4 | ... | 2 | ... |
| CO5 | 3 | 2 | 1 | ... | 3 | 3 | 2 |

| I.K. GUJRAL PUNJAB TECHNICAL UNIVERSITY DEPARTMENT OF CHEMICAL SCIENCES | | | | |
|--|---|------------|------------|------------------|
| Course Name | M.Sc. Chemistry | | | |
| Subject Code: | CHL505A-18 | | | |
| Subject Title: | BIOPHYSICAL CHEMISTRY | | | |
| Contact Hours: | L:3 | T:0 | P:0 | Credits:3 |
| Examination Duration (hours) | 3 | | | |
| Objective(s): | Biophysical chemistry is an interdisciplinary subject which enables students to have an insight of physico-chemical properties of bio macromolecules by using principles & laws governing physics & chemistry and have an understanding of various biological processes. Therefore the objective of teaching this subject of Biophysical Chemistry is to prepare the students who are interested in having their careers in Bioengineering, Molecular Medicine, Biochemistry and Molecular Biology, Biophysics. | | | |

Details of the Course

| Unit | Contents | Contact Hours |
|------|--|---------------|
| I | Biological macromolecules: An introduction to the configuration and conformation of macromolecules; molecular interactions in macromolecular structure, Structure of Proteins (1 ⁰ , 2 ⁰ , 3 ⁰ and 4 ⁰) & Nucleic acids. | 6 |
| | Water: Weak interaction in aqueous systems, interactions of molecules with water, ionization in weak acids and bases; buffering against pH changes in biological systems; water as reactant; and role of water in maintaining the native structure of biopolymers. | 5 |
| II | Bioenergetics and thermodynamics: Biological energy transformations and the laws of thermodynamics; concepts of standard free energy, entropy, enthalpy, and chemical potential changes in biochemical reactions; relationship between equilibrium constant and standard free energy; the effect of temperature and pH on standard free energy; free energy changes associated with hydrolytic and redox (electron transfer) reactions in biological systems. | 12 |
| III | Techniques to study structure and function of biomolecules: An overview of UV-Visible, fluorescence, and circular dichroism (CD) spectroscopy; ultracentrifugation, sedimentation velocity and equilibrium determination of molecular weights; Diffraction and light scattering techniques; and nuclear magnetic resonance. | 12 |

| | | |
|----|--|----|
| IV | Study of the behaviour of biomolecules: Ligand interactions at equilibrium and its kinetics; conformational transitions of polypeptides and proteins: helix-coil transition and reversible protein folding; nucleic acid structural transitions; and membrane equilibria and transport. | 10 |
|----|--|----|

Reference Books

| S.No. | Author(s) | Title of the Book | Publisher/Year |
|-------|---|--------------------------------------|--------------------------------------|
| 1. | Kensel E. Van Holde, W. Curtis Johnson & P. Shing Ho. | Principles of Physical Biochemistry | Pearson Prentice Hall, USA (2006) |
| 2. | James P Allen | Biophysical Chemistry | John Wiley & Sons, USA (2008) |
| 3. | H R Horton, L A Moran, K G Scrimgeour, M D Perry & J D Rawn | Principles of Biochemistry | Pearson Prentice Hall, USA (2006) |
| 4. | D. L. Nelson & M.M. Cox | Lehninger Principles of Biochemistry | WH Freeman Company, New York. (2008) |

Course Outcomes & Mapping

| | | | | | | | |
|---|--|------|------|------|------|------|------|
| At the end of the course, the student will be able to | | | | | | | |
| CO1. | Learn different interactions account for formation of different structures of Biological Macromolecules in living systems. | | | | | | |
| CO2. | Learn applications of thermodynamics in biological systems such as macromolecules in solution and conformation equilibria. | | | | | | |
| CO3. | Describe how kinetic factors influence the biochemical reactions. | | | | | | |
| CO4. | Explain biophysical and chemical methods that are used to study the regulation and function of biomolecules. | | | | | | |
| CO5. | Learn to apply various analytical techniques to understand structural & functional properties of biomolecules. | | | | | | |
| | PSO1 | PSO2 | PSO3 | PSO4 | PSO5 | PSO6 | PSO7 |
| CO1 | 3 | 2 | 4 | 2 | 3 | 4 | 5 |
| CO2 | 3 | 3 | 4 | - | 3 | 5 | 5 |
| CO3 | 3 | 2 | 4 | - | 3 | 5 | 5 |
| CO4 | 3 | 2 | 4 | - | 3 | 5 | 5 |
| CO5 | 2 | 2 | 4 | - | 4 | 4 | 5 |

| I.K. GUJRAL PUNJAB TECHNICAL UNIVERSITY DEPARTMENT OF CHEMICAL SCIENCES | | | | |
|--|---|------------|------------|------------------|
| Course Name | M.Sc. Chemistry | | | |
| Subject Code: | CHL 505B-18 | | | |
| Subject Title: | MEDICINAL CHEMISTRY | | | |
| Contact Hours: | L:4 | T:0 | P:0 | Credits:4 |
| Examination Duration (hours) | 3 | | | |
| Objective(s): | The aim and objective of this course is to familiarize students with the basic concept of Medicinal Chemistry. Emphasis will be made on the SAR of various drugs such as Antimicrobial, antihelmenthics, antifungal and their mode of actions. The commercial synthesis of representative of such drugs will also be discussed. | | | |

Details of the Course

| Unit | Contents | Contact Hours |
|-------------|---|----------------------|
| I | <p>Antibacterial Drugs: Structure, stereochemistry, Mode of action, Structure activity relationships, specific clinical applications of following classes of pharmaceuticals with synthetic/commercial route to the indicated examples. Penicillines, Cephalosporins, Tetracyclines, Aminoglycosides, Chloramphenicol, Macrolides, Lincomycins, Polypeptides antibiotics, Polyene antibiotics. Sulfonamides and Sulfones fluoroquinolones, Trimethoprim and other unclassified antibiotics. Antimycobacterials: Sulfanilamides, p-Aminosalicylic acid derivatives, Thioamides, Thiourea, derivatives, Thiosemicarbazones, Isoniazid, Kanamycin sulfate, Capreomycin, Rifaampin, Pyrazinamide, Anthionamide, Clofazimine, Cyclosporin, Dapsone, Sulfazem.</p> <p>Commercial synthetic/semi-synthetic routes to: 6-aminopenicillanic acid, ampicillin, amoxycillin, production of penicillin, 7-aminocephalosporanic acid, cephalexin, ceftizoxime, cefaclor, cephslothin, Tetracyclins: doxycycline, nalidixic acid, sulfadiazine, Norflaxacin, Ciproflexacin, O-flaxacin, Amiflaxacin, Difloxacin, Chloramphenicol, Nitrofluranton, Sulfamethyoxazole, Acetysulfoxiazole, Trimethoprim.</p> | 10 |
| II | <p>Antiamoebic and Antiprotozoal Drugs: Emetine hydrochloride, 8-Hydroxyquinoline, Iodochlorohydroxyquinol, Metronidazole, Diloxanide furoate, Bilamical hydrochloride, Hydroxystilbamidine isothionate, Pentamidine isothionate, Nifurtimox, Suramin sodium, Carbarsone, Glycobiarsol, Melarsoprol, Sodium stibogluconate, Dimercaprol, Diethylcabamazine citrate, Centarsone, Acetarsone, Antimony potassium tartarate, Bismuth sodium thioglycollate,</p> | 15 |

| | | |
|-----|---|----|
| | Sulphonamide, Stibiophen. Bismuth sodium thioglycollamate, Furazolidone. Commercial synthetic routes to: Metronidazole, ronidazole, flunidazole, iodoquinol, nifurfimox, benzindazole, tryparsamide. | |
| III | a. Antimalarial Drugs: Cinchona alkaloids, 4-Aminoquinolines, 8-Aminoquinolines, 9-Aminoacridines, Biguanides, Pyrimidines and Sulfones, Mefloquine, Sulfonamides. Commercial synthetic routes to: Chloroquine, pamaquine, primaquine, proguanil, Amodiaquine, Mefloquine, Pyremethamine, Sontoquine. b. Anthelmintic Drugs: Introduction, Tetrachloroethylene, Piperazines, Gentian violet, Pyrvinium pamoate, Thiabendazole, Mabendazole, baphenium hydroxynaphthoate, Dichlophen, Niclosamide, Levamisole hydrochloride, Tetramisole, Niridazole, Biothional, Antimonypotassium tartarate, Stibiophen, Sodium Stibiocaptate. | 10 |
| IV | Antifungal Drugs: Fatty acids and their derivatives (Propionic acid, zinc propionate, sodium caprylate, zinc caprylate, undecylenic acid, Zinc undecylenate, Triacetin), Salicylanilids, Salicyclic acid, Tolnaftate, pchloromethoxylenol, Acrisocrin, Fluconazole, Itraconazole, Haloprogin, Clotrimazole, Econazole, Miconazole, Ketoconazole, Flucytosine, Griseofulvin, Polyene antibiotics (Nystatin, Amphoetericin-B), Chlorophenesin, Dithranol. Commercial synthetic routes to: Miconazole, Clotrimazole, Econazole, Fluconazole, Griseofulvin, Ketoconazole, Naftidine, Tolnaftate, Flucytosin. | 10 |

Reference Books

| S.No. | Author(s) | Title of the Book | Publisher |
|-------|--------------------------------------|--|--|
| 1 | W.O. Foye, T.L. Lamke, D.A. Williams | Principles of Medicinal Chemistry, 5 th Edition, | Lippincott Williams and Wilkins, 2002 |
| 2 | R.F. Deorge | Wilson and Gisvolds Textbook of Organic Medicinal and Pharmaceuticals Chemistry, 8 th ed. | J.B. Lippincott Company, Philadelphia, 1982. |
| 3 | B.G. Reuben and H.A. Wittcoff | Pharmaceutical Chemicals in Perspective | John Wiley & Sons, New York, 1989. |

Course Outcomes and Mapping

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

- CO1.** Understand the need of Medicinal Chemistry in curing various ailments.
- CO2.** Study the concept of Antimicrobial and Anti-protozoal drugs.
- CO3.** Study the SAR of Antimicrobial and Anti-protozoal drugs.
- CO4.** Understand the total synthesis of Antimicrobial and Anti-protozoal drugs.
- CO5.** Understand the various diseases cured by Antimicrobial and Anti-protozoal drugs.

| | | | | | | | |
|--|--|------------|------------|------------------|------|------|------|
| | PSO1 | PSO2 | PSO3 | PSO4 | PSO5 | PSO6 | PSO7 |
| CO1 | 5 | 3 | 3 | 4 | 1 | 4 | 4 |
| CO2 | 5 | 1 | 3 | 2 | 1 | 3 | 3 |
| CO3 | 4 | 2 | 3 | 3 | 1 | 4 | 4 |
| CO4 | 3 | 1 | 3 | 2 | 1 | 2 | 2 |
| CO5 | 4 | 1 | 3 | 2 | 1 | 2 | 2 |
| I.K. GUJRAL PUNJAB TECHNICAL UNIVERSITY | | | | | | | |
| DEPARTMENT OF CHEMICAL SCIENCES | | | | | | | |
| Course Name | M.Sc. Chemistry | | | | | | |
| Subject Code: | CHL505C-18 | | | | | | |
| Subject Title: | ADVANCED FUNCTIONAL MATERIALS | | | | | | |
| Contact Hours: | L:4 | T:0 | P:0 | Credits:4 | | | |
| Examination Duration (hours) | 3 | | | | | | |
| Objective(s): | To introduce the students in the area of various functionalized materials, their synthesis and their properties with emphasis to their applications. | | | | | | |

| Unit | Contents | Contact Hours |
|-------------|--|----------------------|
| I | 3-D Carbon-rich p-Systems – Nanotubes and Segments: Functionalization of Carbon Nanotubes, Introduction to Carbon Nanotubes – A New Carbon Allotrope, Functionalization of Carbon Nanotubes, Covalent Functionalization, Halogenation of Carbon Nanotubes, Fluorination of Carbon Nanotubes, Chlorination of Carbon Nanotubes, Bromination of MWCNTs, Chemical Derivatization of “Fluoronanotubes”, Oxidation of CNTs – Oxidative Purification, Carboxylation of CNTs, Defect Functionalization–Transformation of Carboxylic Functions, Hydrogenation of Carbon Nanotubes, Addition of Radicals, Addition of Nucleophilic Carbenes, Sidewall Functionalization Through Electrophilic Addition, Functionalization Through Cycloadditions, Addition of Carbenes, Addition of Nitrenes | 12 |
| II | Cyclophenacene Cut Out of Fullerene:- Introduction, Synthesis of [10]Cyclophenacene β -Conjugated Systems from [60]Fullerene, Synthetic Strategy, Synthesis and Characterization of [10]Cyclophenacenes, Structural Studies and Aromaticity of [10]Cyclophenacene, Synthesis of Dibenzo-fused Corannulenes. Strategic Advances in Chromophore and Materials Synthesis Introduction, Oligomers with a Tetrahedral Core Unit, Oligomers with a Tetrasubstituted Benzene Core, Oligomers with a Tetrasubstituted Biaryl Core. | 11 |
| III | Advanced Biodegradable Organic Polymers: Introduction, Synthesis of Biodegradable Polymers by Polycondensation, General Polycondensation Technique, Post Polycondensation Technique, Chain-Extension Technique, Enzyme-Catalyzed Polycondensation, Synthesis of Biodegradable Polymers by ring- | 11 |

| | | |
|----|--|----|
| | opening polymerization, Monomers, Polymerization with Metal Catalysts, Polymerization Using Metal-Free Organic Catalysts | |
| IV | Antimicrobial Biopolymers: Introduction, Biopolymers, ϵ -Poly-L-Lysine, Chitin and Chitosan, Synthetic Biodegradable Polymers, Quaternary Polymers, Polyethylenimine, Antimicrobial Peptide Mimics, Metal Loading, Silver, Magnesium, Zinc, Titanium, Assessment of Antimicrobial/Antifungal Testing Methods | 11 |

Reference Books

| S.No. | Author(s) | Title of the Book | Publisher/Year |
|-------|--|--|----------------|
| 1 | Thomas J.J. Müller (Editor), Uwe H.F. Bunz (Editor) | Functional Organic Materials Volume-I | Wiley-VCH |
| 2 | Hee-Gweon Woo (Editor), Hong Li (Editor) | Advanced Functional Material | Springer |

Course Outcomes and Mapping

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

- CO1.** Understand the basic concepts and formation of various carbon nano tubes and its functionalizations.
- CO2.** Know the types and structure of functionalized fullerenes.
- CO3.** Learn the common and important synthesis methods, structure and composition of organic polymers and its properties and applications.
- CO4.** Understand the synthesis and applications of Antimicrobial biopolymers.
- CO5.** Learn the various approaches for the synthesis of nanoscale materials/nanoparticles and their properties and applications.

| | PSO1 | PSO2 | PSO3 | PSO4 | PSO5 | PSO6 | PSO7 |
|-----|------|------|------|------|------|------|------|
| CO1 | 2 | 2 | 4 | 2 | 2 | 2 | 2 |
| CO2 | 1 | 3 | 4 | 2 | 3 | 3 | 4 |
| CO3 | 4 | 3 | 5 | 4 | 3 | 4 | 4 |
| CO4 | 1 | 3 | 4 | 2 | 2 | 3 | 2 |
| CO5 | 3 | 3 | 4 | 4 | 3 | 5 | 4 |

| I.K. GUJRAL PUNJAB TECHNICAL UNIVERSITY DEPARTMENT OF CHEMICAL SCIENCES | | | | |
|--|--|------------|------------|------------------|
| Course Name | M.Sc. Chemistry | | | |
| Subject Code: | CHP506-18 | | | |
| Subject Title: | ADVANCED CHEMISTRY LAB-II | | | |
| Contact Hours: | L:0 | T:0 | P:6 | Credits:3 |
| Examination Hours: | 6 | | | |
| Objective(s): | To provide students practical knowledge and skills about various topics taught in theory class of physical chemistry | | | |

Details of the Course

| Unit | Contents |
|------|--|
| I | <p>Any 10 experiments to be performed out of the following:</p> <ol style="list-style-type: none"> 1. Preparation and study of Hardy – Schulze's rule for arsenious sulphide / Ferric hydroxide sols. 2. Verify the Freundlich adsorption isotherm for adsorption of CH_3COOH from its aqueous solution by activated charcoal. 3. Composing a phase diagram for three component system. 4. Determination of distribution coefficient of I_2 between CCl_4 and H_2O. 5. To show that benzoic acid dimerises in benzene by distribution method. 6. Determination of degree of hydrolysis of aniline hydrochloride at room temperature and hence hydrolysis constant of the salt. 7. Determination of pH of various mixtures of sodium acetate and acetic acid in aqueous solutions and hence determine the dissociation constant of the acid. 8. Determination of equilibrium constant of a reaction potentiometrically. 9. To construct a calibration curve for quinhydrone electrode and thus determine its standard reduction potential. 10. Determination of dissociation constant of a dibasic acid potentiometrically. 11. Determination of composition of KCl-KBr mixtures by potentiometric titration against silver nitrate solution. 12. Determination of acid and basic dissociation constants of an amino acid and hence the iso- electric point of the acid. 13. Titration of a mixture of Chloride and Iodide with AgNO_3 potentiometrically. |

| | |
|----|--|
| | 14. Titration of Phosphoric acid solution with NaOH using quinhydrone electrode. 15. Determination of Solute species in a phosphate mixture potentiometrically. |
| II | Any 5 experiments to be performed out of the following: <ol style="list-style-type: none"> 1. Separation of a mixture of amino acids using thin layer chromatography. 2. Isolation and quantitation of DNA from onion. 3. Separation of DNA using gel electrophoresis (agarose). 4. Isolation, detection, and quantitation of protein (casein) from milk. 5. Osmosis and diffusion through semipermeable membrane. 6. Estimation of DNA quantity using UV-Vis spectrophotometer. 7. DNA/ligand interaction (Scatchard plot) using UV-Vis spectrophotometer. 8. Serum albumin/ligand interaction using UV-Vis spectrophotometer |

Reference Books

1. Advanced Practical Physical Chemistry by J.B. Yadav.
2. Findlay's Practical Physical Chemistry.
3. Safety-Scale Laboratory Experiments for Chemistry for Today, S L Seager and M R Slabaugh, Brooks/Cole Laboratory Series for General, Organic, and Biochemistry, VII edition, Brooks/Cole, 2010

Course Outcomes and Mapping

| | | | | | | | |
|--|--|------|------|------|------|------|------|
| At the end of the course, the students will be able to | | | | | | | |
| CO1. | Emphasize the importance of different techniques used for titration viz. potentiometry, pHmetry and amperometry . | | | | | | |
| CO2. | Correlate the theoretical and practical aspects and know about the limits of the experimental error. | | | | | | |
| CO3. | Determine the various physical parameters for the various problems under study which in turn will enhance their problem solving and analytical skills. | | | | | | |
| CO4. | Verify various laws studied in the theory part. | | | | | | |
| | PSO1 | PSO2 | PSO3 | PSO4 | PSO5 | PSO6 | PSO7 |
| CO1 | 1 | 4 | 4 | 3 | 5 | 5 | 3 |
| CO2 | 2 | 4 | 5 | 3 | 5 | 2 | 4 |
| CO3 | 2 | 5 | 5 | 2 | 4 | 3 | 5 |
| CO4 | 2 | 4 | 5 | 1 | 4 | 2 | 5 |

SEMESTER-IV

| I.K. GUJRAL PUNJAB TECHNICAL UNIVERSITY DEPARTMENT OF CHEMICAL SCIENCES | | | | |
|--|--|------------|------------|------------------|
| Course Name | M.Sc. Chemistry | | | |
| Subject Code: | CHL511-18 | | | |
| Subject Title: | ADVANCED ORGANIC CHEMISTRY-II | | | |
| Contact Hours: | L:4 | T:0 | P:0 | Credits:4 |
| Examination Duration (hours) | 3 | | | |
| Course Objective(s): | The objective of this course is to familiarize the students about the concept of asymmetric synthesis, and its applications in organic synthesis. Another objective of the course is to make student understand the use of disconnection approach in Organic Synthesis. The use of organometallic reagent in organic synthesis will also be covered to give an emphasis on importance of organometallic reagents in organic synthesis. | | | |

Details of the Course

| Unit | Contents | Contact Hours |
|-------------|--|----------------------|
| I | Asymmetric synthesis: Analytical methods for determination of enantiomeric purity – GC, HPLC and NMR. Natural sources of chiral starting materials, classification and methods of formation of new chiral compounds. Non enzymatic methods of asymmetric synthesis: Methods of asymmetric synthesis using naturally occurring chiral compounds, chiral auxiliaries and their functions, Diels – Alder cycloadditions, Michael reaction and addition to carbonyl compounds. Cram's rule and Felkin – Ahn model. Asymmetric oxidation and reductions. | 10 |
| II | Disconnection approach and Strategies for disconnection approach: An introduction to synthons and synthetic equivalents, disconnection approach, functional group interconversions, The importance of the order of events in organic synthesis, chemoselectivity, reversal of polarity, cyclisation reactions, protecting groups, stereoselectivity, regioselectivity, use of acetylenes, carbonyl condensation and control in carbonyl condensation, use of aliphatic nitro compounds, radical reaction, | 15 |

| | | |
|-----|---|----|
| | reconnections, ring synthesis (3,4,5 and 6 membered), rearrangements, use of ketenes. | |
| III | One group disconnections: One group C-X and C-C disconnections (alcohol and carbonyl compounds) Two group disconnections: Two group C-X disconnections in 1,2-difunctionalized compounds, 1,3-difunctionalized compounds and α,β -unsaturated carbonyl compounds, 1,4-difunctionalized compounds, 1,5-difunctionalized compounds and 1,6-difunctionalized compounds. | 10 |
| IV | Organometallic Catalysis in organic synthesis: Fundamental reaction steps of transition metal catalysed reaction. oxidative-addition reactions, elimination reactions, cleavage of C-H bonds, migration reaction, insertion reaction, Hydrogenation reactions, hydrosilylation reactions, hydroformylation of unsaturated compounds, carbonylation reactions, C-C cross coupling and related reaction, alkene and alkyne metathesis, C-H activation using metal salts, Suzuki reaction, Heck reaction, Negishi coupling, Stille reaction, Sonogashira coupling reactions. | 10 |

Reference Books

| S.No. | Author(s) | Title of the Book | Publisher |
|-------|---|--|--|
| 1 | Francis A. Carey and Richard J. Sundberg | Advanced Organic Chemistry Vol. A and Vol. B, fourth Edition | Kluwer Academic publishers, New York 2002 |
| 2 | Jerry March | Organic Reaction Mechanism | John Wiley Ed. 5, 2002 |
| 3 | W. Carruthers | Some Modern Methods of Organic Synthesis, IV Edition | Cambridge University Press, 2004 |
| 4 | H.O. House | Modern Synthetic Reactions | The Benjamin Cummings Publishing Company, London, 1972 |
| 5 | Guo-Qiang Lin Yue-Ming Li Albert S. C. Chan | Principles and Applications of Asymmetric Synthesis | John Wiley & sons, |
| 6 | J. Furhop and G. Penzillin, | Organic Synthesis-concept, methods and starting materials | Verlage VCH. |
| 7 | Stuart Warren, Paul Wyatt, | Organic Synthesis: The Disconnection Approach | Wiley; 2nd Edition edition. |

Course Outcomes and Mapping

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

- CO1.** Explain the concept of asymmetric synthesis.
- CO2.** Understanding the physical methods in analyzing the asymmetry.
- CO3.** Understand the methodological concept of connection disconnection in organic synthesis.

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|-------------|--|------|------|------|------|------|------|
| CO4. | Emphasize the role of various organometallic complexes in Organic Synthesis. | | | | | | |
| CO5. | Explore the use of various metals in organic synthesis | | | | | | |
| | PSO1 | PSO2 | PSO3 | PSO4 | PSO5 | PSO6 | PSO7 |
| CO1 | 2 | 4 | 4 | 2 | .. | 1 | 2 |
| CO2 | 2 | 4 | 4 | 1 | .. | 1 | 2 |
| CO3 | 2 | 4 | 4 | 1 | .. | 1 | 1 |
| CO4 | 2 | 4 | 4 | 1 | .. | 1 | 4 |
| CO5 | 2 | 4 | 4 | 1 | .. | 1 | 4 |

| I.K. GUJRAL PUNJAB TECHNICAL UNIVERSITY DEPARTMENT OF CHEMICAL SCIENCES | | | | |
|--|---|------------|------------|------------------|
| Course Name | M.Sc. Chemistry | | | |
| Subject Code: | CHL 512A-18 | | | |
| Subject Title: | ADVANCED PHYSICAL CHEMISTRY | | | |
| Contact Hours: | L:4 | T:0 | P:0 | Credits:4 |
| Examination Duration (hours) | 3 | | | |
| Objective(s): | The objective of this course is to provide an introduction to few advanced topics in physical chemistry like the chemistry of colloids, macromolecules and the latest electroanalytical techniques, focussing especially on their application part. | | | |

Details of the Course

| Unit | Contents | Contact Hours |
|------|--|---------------|
| I. | Colloidal State: Classification of colloids, charge and stability of colloidal dispersions, Hardy-Schulze Law, gold number, electrical properties of colloids, zeta-potential, electrophoresis and electroosmosis, emulsions and their classification, gels and their classification, thixotropy. Micelles, Surface active agents, Classification of surface active agents, Micellization, Hydrophobic interaction, Critical micellar concentration (cmc), Factors affecting the concentration of surfactants, Counter-ion binding of micelle, Thermodynamics of micellization, Applications. | 11 |
| II. | Polymers: Types of polymers, regular and irregular polymers, electrically conducting polymers, synthesis of polymers by chain and step reaction polymerization, physical properties of solid polymers (crystallinity, plasticity & elasticity) vulcanization of rubbers, molecular mass determination by osmometry, viscometry, light scattering and ultracentrifuge methods, number and mass average molecular masses, polymer solutions, factors affecting the solubility of polymers. | 12 |
| III. | Voltammetric Techniques-I: Linear sweep voltammetry; voltammetric electrodes, voltammograms. Hydrodynamic | 10 |

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|-----|--|----|
| | Voltammetry; concentration profiles at electrode surfaces, voltammetric currents, current voltage relationships, voltammograms for mixtures, Applications; voltammetric detectors, amperometric sensors, amperometric titrations. Differential pulse voltammetry. | |
| IV. | Voltammetric Techniques-II: Polarography: principle, instrumentation and Applications, advantages and disadvantages of DME. Cyclic Voltammetry: Electrode used in cyclic voltammetry, electrochemical mechanism, Eads mechanism (Adsorption mechanism), Butler-volmer equation, Reversible one electron transfer. | 12 |

Reference Books

| S.No. | Author(s) | Title of the Book | Publisher/Year |
|-------|-------------------------------|--|---|
| 1. | R.J. Young and P.A.Lovell | Introduction to Polymers | Chapman and Hall London, 2nd ed., New Delhi (2004) |
| 2. | F.W. Jr. Billmeyer | Text book of polymers science | Wiley-Interscience, 3 rd ed. (1984) |
| 3. | D. Myers | Surfactant Science and Technology | VCH Publishers (1988) |
| 4. | P.J. Flory | Principles of polymer chemistry | Cornell Univ. Press, Ithaca (Indian Print 2006) |
| 5. | M.J. Rosen | Surfactants and Interfacial Phenomena | John Wiley & Sons (1989) |
| 6. | P.H. Reiger | Electrochemistry | Prentice-Hall, New Jersey (1994) |
| 7. | D.R. Crow | Principles and Applications of Electro-chemistry | Blackie academic, Glasgow (1988) |
| 8. | Bard & Faulkner | Electrochemical Methods: Fundamentals and Applications | |
| 9. | C.M.A. Brett and A.M.O. Brett | Electrochemistry: Principles, Methods and Applications | Oxford Uni. Press (1993) |

Course Outcomes and Mapping

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|---|--|
| At the end of the course, the student will be able to | |
| CO1. | Understand major aspects of chemical terminology related to surface science, polymers and electrode processes. |
| CO2. | Develop insights in the micelle formation process and emphasize its application in daily life. |
| CO3. | Know about polymers in detail. |

| | | | | | | | |
|-------------|---|------|------|------|------|------|------|
| CO4. | Correlate various types of voltammetric techniques and their importance in sensing field. | | | | | | |
| | PSO1 | PSO2 | PSO3 | PSO4 | PSO5 | PSO6 | PSO7 |
| CO1 | 2 | 4 | 5 | ... | 3 | 2 | 2 |
| CO2 | 2 | 3 | 5 | 2 | 2 | 2 | 2 |
| CO3 | 3 | 2 | 4 | 2 | ... | 3 | 2 |
| CO4 | 2 | 3 | 3 | ... | 2 | 3 | 3 |

| I.K. GUJRAL PUNJAB TECHNICAL UNIVERSITY DEPARTMENT OF CHEMICAL SCIENCES | | | | |
|--|--|------------|------------|------------------|
| Course Name | M.Sc. Chemistry | | | |
| Subject Code: | CHL512B-18 | | | |
| Subject Title: | CHEMICAL TOXICOLOGY | | | |
| Contact Hours: | L:4 | T:0 | P:0 | Credits:4 |
| Examination Duration (hours) | 3 | | | |
| Objective(s): | The course objective is to make students familiar with basic principles of Chemical Toxicology including aspects of exposure, toxicity & risks assessment of chemicals in the environment so that they can understand hazards & risks associated with them and handle them safely. | | | |

Details of the Course

| Unit | Contents | Contact Hours |
|------|--|---------------|
| I | Introduction to Toxicology: Risk Assessment & Management Definitions, Scope & Relationship with other sciences, History and milestones in Toxicological Sciences; Sources of Toxic Compounds; Exposure Classes (Air Pollutants, Water & Soil Pollutants, Occupational Pollutants), Use Classes (Metals, Agrochemicals, Food additives and Toxins). Process of Risk assessment, Hazard Identification & Characterization (Types & Source of Information, Dose response, Dose Effect, Human & Environmental Exposure); Risk Evaluation & Management Process, Risk Considerations, Criteria for Risk Evaluations (Human health & Environment), Risk Management. | 12 |
| II | Toxicokinetics Absorption, Distribution, Metabolism (Phase-I, Phase-II Reactions & Activation Enzymes, Reactive Metabolites; Nature & Stability of Reactive Metabolites, Fate of Reactive Metabolites and factors affecting their toxicity) and Elimination of Toxicants. | 8 |
| III | Environmental Toxicology | 6 |

| | | |
|----|--|---|
| | Environmental Persistence, Bioaccumulation and Toxicity of Toxicants. Sources of Toxicants: Transportation Processes, Equilibrium Partitioning, Transformation Processes. | |
| IV | Safe Handling of Chemicals Introduction, Legislation, Toxicological Reactions (Corrosion, Organic Compounds, Biological Materials, Allergens, Pharmaceuticals & Radionuclides), Good Laboratory Practices, Health & Safety, Protocols & Procedures | 4 |

Reference Books

| S.No. | Author(s) | Title of the Book | Publisher/Year |
|-------|---|--|-----------------------------------|
| 1 | John H. Duffus & Howard G.J. Worth | Fundamental Toxicology | Royal Society of Chemistry (2006) |
| 2 | Ernst Hodgson | A Text Book of Modern Technology | John Wiley & Sons (2004) |
| 3 | Poisoning & Toxicology Handbook | Jerrold B Leikin & Frank P. Pauloczek | Informa Healthcare USA (2008) |
| 4 | Environmental Toxicants: Human Exposures & Their Health Effects | Morton Lippman | John Wiley & Sons (2009) |
| 5 | Handbook on the Toxicology of Metals | G.A. Nordberg, B.A. Fowler, M. Nordberg & Lars Friberg | Academic Press (2005) |

Course Outcomes and Mapping

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

- CO1.** Acquired broad knowledge of environmental toxicants & their effects on the physiological systems.
- CO2.** Describe basic toxicological principles and how different chemicals are taken up by, processed in and eliminated from the body.
- CO3.** To synthesize and apply concepts from various other disciplines in environmental & chemical toxicology.
- CO4.** Apply different toxicological frameworks within the professional disciplines and have awareness about different risk assessment criteria.
- CO5.** Learn safe handling of chemicals in the laboratory.

| | PSO1 | PSO2 | PSO3 | PSO4 | PSO5 | PSO6 | PSO7 |
|-----|------|------|------|------|------|------|------|
| CO1 | 4 | 3 | - | 4 | 3 | 5 | 4 |
| CO2 | - | 3 | 3 | 3 | 3 | 4 | 4 |
| CO3 | 3 | 5 | 5 | 5 | 3 | 4 | 4 |
| CO4 | 3 | 3 | 3 | 3 | - | 4 | 3 |
| CO5 | 5 | - | 2 | - | 4 | - | - |

| I.K. GUJRAL PUNJAB TECHNICAL UNIVERSITY DEPARTMENT OF CHEMICAL SCIENCES | | | | |
|--|--|------------|------------|------------------|
| Course Name | M.Sc. Chemistry | | | |
| Subject Code: | CHL512C-18 | | | |
| Subject Title: | SUPRAMOLECULAR CHEMISTRY | | | |
| Contact Hours: | L:4 | T:0 | P:0 | Credits:4 |
| Examination Duration (hours) | 3 | | | |
| Objective(s): | To impart in depth knowledge of non-covalent interactions in supramolecular systems and their applications | | | |

Details of the Course

| Unit | Contents | Contact Hours |
|-------------|---|----------------------|
| I | Host-Guest Chemistry: Definition-Supramolecular chemistry, Host-guest and Self-assembly; Selectivity, Preorganization and Complementarity of binding sites, Chelate ring size effect, Donor group and orientation; Binding constants, Thermodynamic and kinetic selectivity; Solvent effects and Non-covalent interactions | 11 |
| II | Solution Host-Guest Chemistry and Ion Recognition: Macrocyclic vs acyclic hosts, Templates effect and High dilution synthesis; Cation recognition: Crown ethers, Lariat ethers, Podands, Cryptands, Spherands, Calixarenes, Siderophore, Inclusion compounds, Molecular clefts and Tweezers; Anion recognition: Challenge in anion receptor chemistry, Charged and neutral receptors, contact ion pairs, cascade complex, remote anion and cation binding sites. | 12 |
| III | Basic concepts of self-assembly and classification: 10Hrs Self-Assembly in Synthetic Systems: Template effects in synthesis, Self-Assembly with covalent modification, A Thermodynamic Model: Self-assembly of zinc porphyrin complexes, Cooperativity and the extended site binding model | 12 |

| | | |
|----|---|----|
| | Self-Assembly in biological Systems: Biological self-assembled fibres and layers, Amyloids, Actins and Fibrin, Bacterial S-Layers, Single molecule self-assembly: Proteins and Foldamers, Strict Self-Assembly: The Tobacco Mosaic Virus and DNA | |
| IV | Catenanes and Rotaxanes: Statistical approaches to catenanes and rotaxanes, π - π and Hydrogen bonded rotaxanes and catenanes, Metal and auxiliary linkage approaches to catenanes and rotaxanes. Molecular Devices: , Logic gate, Molecular switches, Molecular motor. | 10 |

Reference Books

| S.No. | Author(s) | Title of the Book | Publisher/Year |
|-------|---------------------------|---|----------------|
| 1 | J. W. Steed, J. L. Atwood | Supramolecular Chemistry, Second edition | 2009, Wiley |
| 2 | Jean-Marie Lehn | Supramolecular Chemistry | 1995, Wiley |
| 3 | K. Ariga, T. Kunitake | Supramolecular chemistry-fundamental and applications | 2006, Springer |

Course Outcomes and Mapping

| <p>The students will acquire knowledge of</p> <p>CO1. To learn the fundamental concepts of supramolecular chemistry such as Host-guest chemistry/ self-assembly.</p> <p>CO2. Various kinds of non-covalent interactions occurring in supramolecular systems.</p> <p>CO3. Molecular recognition and nature of bindings involved in biological systems.</p> <p>CO4. Structure of supramolecules of various types in solution and solid state.</p> <p>CO5. Applications of supramolecules in miniaturization of molecular devices.</p> | | | | | | | |
|--|------|------|------|------|------|------|------|
| | PSO1 | PSO2 | PSO3 | PSO4 | PSO5 | PSO6 | PSO7 |
| CO1 | 3 | 1 | 3 | 1 | 4 | 4 | 2 |
| CO2 | 3 | - | 1 | 2 | 1 | 4 | 3 |
| CO3 | 3 | - | 1 | 2 | 1 | 4 | 3 |
| CO4 | 3 | - | 1 | 2 | 1 | 4 | 3 |
| CO5 | 5 | - | 3 | 1 | 1 | 4 | 4 |

| I.K. GUJRAL PUNJAB TECHNICAL UNIVERSITY DEPARTMENT OF CHEMICAL SCIENCES | | | | |
|--|--|------------|------------|------------------|
| Course Name | M.Sc. Chemistry | | | |
| Subject Code: | CHL512D-18 | | | |
| Subject Title: | CHEMISTRY OF NATURAL PRODUCTS | | | |
| Contact Hours: | L:4 | T:0 | P:0 | Credits:4 |
| Examination Duration (hours) | 3 | | | |
| Course Objective(s): | The aim and objective of this course is to make students understand the chemistry of common natural products. The course will involve the structure, chemistry and metabolic pathways involving the common natural products. | | | |

Details of the Course

| Unit | Contents | Contact Hours |
|------|--|---------------|
| I | Terpenoids and Carotenoids: Classification, nomenclature, occurrence, isolation, general methods of structure determination, isoprene rule. Structure determination and synthesis of citral, geraniol, camphor, farsenol, santonin, abetic acid. | 10 |
| II | Alkaloids: Definition, nomenclature and physiological action, occurrence, isolation, general methods of elucidation, degradation, classification based on nitrogen heterocyclic ring, Structure, stereochemistry, synthesis of ephedrine, nicotine, atropine, morphine. | 10 |
| III | Steroids: Occurrence, nomenclature, Isolation, structure determination and synthesis of Cholesterol, bile acids, Androsterone, testosterone, estrone, progesterone. | 10 |
| IV | Secondary Metabolism: (a) Metabolites Derived from Acetate (Polyketide Pathway): Biosynthesis of unsaturated and saturated fatty acids, prostaglandins, polyphenols viz. Orsellinic acid, 6-methylsalicylic | 15 |

| | | |
|--|--|--|
| | acid, usnic acid, penicillic acid, patulin, citrinin, griseofluvin, alizarin, emodin, tetracyclines. (b) Metabolites Derived from Mevalonic Acid Pathway (Terpenes): Biosynthesis of mevalonic acid and the active isoprene units, monoterpenes viz. Citral, geraniol, pinene, camphor, terpineol, thujone, isobornylene, menthol, artemesia alcohol, santolina alcohol, Iridoids, viz. Loganin, iridomyrmecin, secolaganin, sweroside. -bisabolene, γ -cedrene, α Sesquiterpenes, viz. Humulene, ovalicin, juvenile hormone, Diterpenes, viz. Phytol, Sclareol, abietic acid, taxinine. Triterpenes, squalene, lanosterol, cholesterol, cycloartenol, sitosterol, Vitamin D. -carotene, β -carotene, Biological functions of steroids. Biosynthesis of carotenoids, viz. vitamin A | |
|--|--|--|

Reference Books

| S.No. | Author(s) | Title of the Book | Publisher |
|-------|--------------------------------------|---|--|
| 1 | I. L. Finar | Organic Chemistry, Vol. 2. | Longmans Green & Co. 1964 |
| 2 | J. Mann | Secondary Metabolism | Oxford University Press, Oxford, 1980. |
| 3 | Kurt B. G. Torssell, | Natural Product Chemistry - A Mechanistic, Biosynthetic and Ecological Approach | Swedish Pharmaceutical Society, 1997. |
| 4. | by D. Voet, J.G. Voet and C.W. Pratt | Fundamental of Biochemistry | John Willey & Sons Inc., New York, 1999. |
| 5. | A. L. Lehninger | Principles of Biochemistry | CBS Publishers, New Delhi. |

Course outcomes and Mapping

| | | | | | | | |
|--|---|------|------|------|------|------|-------|
| At the end of the course, the student will be able | | | | | | | |
| CO1. | To learn the chemistry and methods to determine structure elucidation of natural products | | | | | | |
| CO2. | To study the chemistry of chemistry of terpenoids and carotenoids | | | | | | |
| CO3. | To study the Chemistry of steroids | | | | | | |
| CO4. | To study the chemistry of v metabolic processes involving such biochemicals | | | | | | |
| CO5. | To understand the role of such natural products in living systems | | | | | | |
| | PSO1 | PSO2 | PSO3 | PSO4 | PSO5 | PSO6 | P2SO7 |
| CO1 | 5 | 3 | 3 | 4 | 1 | 4 | 4 |
| CO2 | 5 | 1 | 3 | 2 | 1 | 3 | 3 |
| CO3 | 4 | 2 | 3 | 3 | 1 | 4 | 4 |
| CO4 | 3 | 1 | 3 | 2 | 1 | 2 | 2 |

| | | | | | | | |
|-----|---|---|---|---|---|---|---|
| CO5 | 4 | 1 | 3 | 2 | 1 | 2 | 2 |
|-----|---|---|---|---|---|---|---|

| I.K. GUJRAL PUNJAB TECHNICAL UNIVERSITY DEPARTMENT OF CHEMICAL SCIENCES | | | | |
|--|--|------------|------------|------------------|
| Course Name | M.Sc. Chemistry | | | |
| Subject Code: | CHL512E-18 | | | |
| Subject Title: | GREEN CHEMISTRY | | | |
| Contact Hours: | L:4 | T:0 | P:0 | Credits:4 |
| Examination Duration (hours) | 3 | | | |
| Objective(s): | 1. To introduce the students of Master class about various concepts of green chemistry and its technologies. 2. The emphasis is on the synthesis of various entities using benign methods of green chemistry (their role and advantages). | | | |

Details of the Course

| Unit | Contents | Contact Hours |
|------|---|---------------|
| I. | Introduction to the Green Chemistry; Historical context: The Greening of Chemistry; Waste: Production, Problems, Prevention; Measuring and Controlling Environmental Performance; planning for the future for reducing carbon in the atmosphere; Emergence of Green chemistry and its environmental impact. | 10 |
| II. | Twelve Principles of green chemistry, concepts, importance and their applications with special emphasis on the use of alternative renewable feedstock (bio-fuels, biomass and their applications in green synthesis of various compounds); Use of innocuous reagents in natural processes; Alternative solvents; Design of the safer chemicals; Designing alternative reaction methodology; Minimizing energy consumption. Sustainable Polymers: The case of polylactide, using CO ₂ and other feedstock. | 10 |

| | | |
|------|---|----|
| III. | Green reactions (Role, advantages and applications): Aqueous phase organic synthesis, Solvent less organic synthesis, Photochemical organic synthesis, PTC catalysed reactions, Microwave induced reactions, Enzymatic transformations, Sonication reactions & reactions in Ionic liquids. | 13 |
| IV. | Green reactions (Role & mechanism): Aldol condensation reaction (solid phase and Ionic liquid synthesis), Baeyer-Villiger oxidation (aqueous phase and solid phase synthesis), Baylis-Hillman Reaction (Microwave synthesis and Ionic liquid synthesis), Biginelli Reaction under Microwave irradiation, Cannizzaro Reaction under sonication, Dakin reaction under ultrasonication, Darzen reaction in PTC, Dieckmann condensation (Polymer supported synthesis), Diels-Alder reaction (in water, ionic liquid, MW and sonication), Photo-Fries rearrangement, Stille coupling in water and SC-CO ₂ , Ullmann reaction under sonication and in aqueous medium, Sonogashira reaction. | 12 |

Reference Books

| S.No. | Author(s) | Title of the Book | Publisher |
|-------|-------------------------------|--------------------------------------|---|
| 1 | Lancaster, M. | Green Chemistry an Introductory Text | Royal Society of Chemistry, Cambridge, UK 2002. ISBM 0-85404-620-8. |
| 2 | Cann, M.C.; Connelly, M.E., | Real World Cases in Green Chemistry | American Chemical Society: Washington DC. 2000. ISBN 0-8412-3733-6. |
| 3 | Anastas, P. T.; Warner, J. C. | Green Chemistry: Theory and Practice | Oxford University Press: New York, 1998. |

Course Outcomes and Mapping

| | | | | | | | |
|---|--|------|------|------|------|------|------|
| At the end of the course, the student will be able to | | | | | | | |
| CO1. | Conceptualize the various syntheses using novel and greener methods. | | | | | | |
| CO2. | Predict the relationships between organic chemical structures and their reactivity in different greener and benign conditions. | | | | | | |
| CO3. | Learn the fundamental and advanced concepts of green chemistry in reaction mechanisms. | | | | | | |
| CO4. | Apply the new methodologies for altering the reactivity patterns of substrates | | | | | | |
| CO5. | Synthesize various molecules using combinations of reactive species in novel conditions. | | | | | | |
| | PSO1 | PSO2 | PSO3 | PSO4 | PSO5 | PSO6 | PSO7 |
| CO1 | 4 | 4 | 4 | 4 | 3 | 5 | 2 |
| CO2 | 3 | 3 | 4 | 2 | 2 | 4 | 2 |
| CO3 | 3 | 3 | 3 | 1 | 3 | 4 | 3 |

| | | | | | | | |
|-----|---|---|---|---|---|---|---|
| CO4 | 4 | 3 | 4 | 2 | 1 | 4 | 2 |
| CO5 | 3 | 4 | 2 | 4 | 2 | 5 | 2 |

| I.K. GUJRAL PUNJAB TECHNICAL UNIVERSITY DEPARTMENT OF CHEMICAL SCIENCES | | | | |
|--|---|------------|------------|------------------|
| Course Name | M.Sc. Chemistry | | | |
| Subject Code: | CHL512F-18 | | | |
| Subject Title: | COMPUTATIONAL CHEMISTRY | | | |
| Contact Hours: | L:4 | T:0 | P:0 | Credits:4 |
| Examination Duration (hours) | 3 | | | |
| Course Objective(s): | Theoretical chemistry lies at the interfaces among chemistry, physics and mathematics. The primary goals of the present course are to provide an overview of the roles that theory plays within the science of chemistry and to introduce the students to the modern day components of theoretical chemistry. | | | |

Details of the Course

| Unit | Contents | Contact Hours |
|------|--|---------------|
| I | The Basics of Quantum Mechanics: Methods for solving Schrodinger equation, Exact Solution, Understanding Energy Surfaces, beyond model problems, normal modes, local modes, transition states, symmetry. An overview of theoretical chemistry: Molecular structure, types of bonding, symmetries groups. | 11 |
| II | Numerical methods: Methods for roots of equations, numerical integration and differential equations, interpolation and extrapolation of data, matrices. Elements of Computer Programming; Introduction to Plotting softwares, Visualization of structures | 11 |

| | | |
|-----|---|----|
| III | Classical Molecular dynamics: Statistical Mechanics of Molecules at or Near Equilibrium, Monte Carlo simulations, Molecular Dynamics Simulations, Theoretical Treatment of Chemical Change and Dynamics, Experimental Probes of Reaction Dynamics, Introduction to some molecular dynamics codes such as GROMAC, PACKMOLE, VMD and CHEMIRA | 11 |
| IV | Ab initio methods and applications: Hartree Methods, Hartree Fock Methods and Geometry Optimization, Non-variational methods, density functional theory and property calculations, Quantum Monte Carlo methods, Introduction to some molecular dynamics codes such as GAUSSIAN | 12 |

Reference Books

| S.No. | Author(s) | Title of the Book | Publisher |
|-------|----------------------------------|--|-----------------------------------|
| 1 | Jack Simons | An Introduction to Theoretical Chemistry, | Cambridge University Press, 2003. |
| 2 | C. J. Cramer | Essentials of Computational Chemistry | Wiley, 2002. |
| 3 | R. D. Levine and R. B. Bernstein | Molecular Reaction Dynamics and Chemical Reactivity, | Oxford University Press, 1997. |
| 4. | A. R. Leach, | Molecular Modeling, 2nd ed | Prentice Hall, 2001. |

Course outcomes and Mapping

| | | | | | | | |
|--|------|------|------|------|------|------|------|
| At the end of the course, the student will be able to | | | | | | | |
| CO6. Bridge the chemistry with modern day physics, material sciences. CO7. Understand theoretical aspects of chemical transformations. CO8. Understand the changes in the physical parameters in chemical reactions. CO9. Rationalize the changes in chemical processes. CO10. Understand the feasibility of the reactions. | | | | | | | |
| | PSO1 | PSO2 | PSO3 | PSO4 | PSO5 | PSO6 | PSO7 |
| CO1 | 3 | 3 | 2 | .. | .. | 3 | 4 |
| CO2 | 2 | 3 | 2 | .. | .. | 4 | 4 |
| CO3 | 2 | 4 | 1 | .. | .. | 3 | 4 |
| CO4 | 2 | 3 | 2 | .. | .. | 2 | 3 |
| CO5 | 2 | 2 | 3 | .. | .. | 3 | 4 |

