Faculty: Science and Technology

Programme: MSc Chemistry (NEPv23)

Programme Educational Objectives (PEOs)

- To mold a generation of youth which can apply the subject knowledge in their life and careers
- To inculcate scientific attitude enriched with a multidisciplinary perspective in the students.
- To update the students with the needs of the industry and society.
- To develop a generation which feels responsible towards the society and the nation

Program Outcomes

PO1: Creative Thinking: Students will be able to think creatively (divergently and convergent) to propose novel ideas in explaining facts and figures or providing new solution to the problems in chemistry. The skills of observations and drawing logical inferences from the scientific experiments will also be developed.

PO2: Interdisciplinary Approach: Students will realize how developments in any science subject helps in the development of other science subjects and vice-versa and how interdisciplinary approach helps in providing better solutions and new ideas for the sustainable developments. Also the knowledge of subjects in other faculties such as humanities, performing arts, social sciences etc. can have greatly and effectively influence which inspires in evolving new scientific theories and inventions.

PO3: Personality Development: Students will imbibe ethical, moral and social values in personal and social life leading to highly cultured and civilized personality. They will also realize that pursuit of knowledge is a lifelong activity and in combination with untiring efforts and positive attitude and other necessary qualities leads towards a successful life.

PO4 Skills in research and industrial field: Students will build a scientific temper and will be able to learn the necessary skills to succeed in research or industrial field. In addition they will acquire the skills in handling scientific instruments, planning and performing in laboratory experiments.

PO5 Communication Skills: Students will develop various communication skills such as reading, listening, speaking, etc., which will help in expressing ideas and views clearly and effectively.

PO6 Environmental monitoring: Students will be able to design a solution to the environmental issues like Global warming, Climate change, Acid rain, Ozone depletion and will create awareness in society.

Program Specific Outcomes:

On completion of M.Sc. Chemistry programme, graduates will be able to:

PSO-1: observe, analyze and interpret chemical phenomena and process

PSO-2: design and develop new molecules/processes with industrial and societal applications

PSO-3: formulate new ideas/concepts in chemical sciences and test them

PSO-4: communicate effectively the principles and practice of chemical sciences

PSO-5: address issues of environment, health and development from a chemical perspective

PSO-6: follow professional ethics in all spheres of activity

PSO-7: function effectively as a member/leader in diverse teams/groups

PSO-8: engage in independent learning in the broadest context of scientific advancement

Employability Potential of MSc (Chemistry):

The scope of M.Sc Chemistry is very diverse when taking into consideration the various avenues that are available for students after graduation. The program MSc (Chemistry) offers the necessary knowledge, skills and attitude to nurture creativity. Some important skills and abilities honed by chemistry learners include:

- Cutting-edge scientific and numerical skills
- Curiosity to understand and solve
- Attention to collect and analyse details
- Patience and determination
- Research and development skills
- Analytical skills
- Use of ICT enabled techniques
- Written and oral communications skills

Apart from the technical and specific skills, a chemistry graduate also acquires fundamental professional skills throughout the degree program to pursue careers not directly related to the field. These skills include:

- Effective listening and communication skills
- Presentation and interaction skills
- Data collection, analysis and reporting skills
- Modern ICT enabled skills
- Aptitude to work proficiently independently or in a team

Equipped with a bunch of requisite knowledge, skills and attitude, a degree in chemistry is recognized as a symbol of quality and commitment by employers within and outside the realm of chemical industries.

The thriving and widely recognized branches of chemistry like Organic, Inorganic, Physical, Analytical, etc. not only expand critical thinking and the ability to understand other scientific and engineering concepts more easily, but also open new horizons to pursue career in different fields.

- Organic chemistry offers research and development of organic materials, modify and study carbon-based materials to develop a product having a specific purpose for wider use. They also accomplish various scientific studies to identify or find applications for compounds for society. Many industries like pharmaceuticals, agriculture, paints, dyes, and many more prefer to employ organic chemists.
- Inorganic chemistry has a greater potential in the fields of metallurgy, synthesis of new materials from different elements, bioinorganic, etc. It focusses on solving the fundamental problems associated with structure of atoms, molecules and their properties. Analytical chemists find their role for toxicology examinations, quality control and assessment, analysis of pharmaceuticals, investigations for forensic analysis, development of equipment, etc.
- Analytical chemists work for a particular private or government laboratory or organization, and also develop particular specialties like food technology, forensics or toxicology, to name a few.
- Physical chemistry enhances critical ability and inculcates problem solving skills among the learners. All industries rely heavily on physical parameters for manufacturing and quality assurance of products

Apart from the core branches of Chemistry, auxiliary branches like medicinal, industrial, petrochemical, geochemistry etc also offers a vast array of employability opportunities. Chemistry graduates apply their skills within the areas of environmental sciences, medical fields, scientific equipment sales, science communication, teaching or academic research, a few to mention. Thus, a degree in chemistry widens numerous prospects and opportunities for a wide variety of careers in many different fields like science, research, business and health care, etc.

Some of the areas of work available to students after the M.Sc Chemistry course are public relations, blog writing, research centres, synthetic labs, chemical firms, academic institutions etc.

The scope of M.Sc Chemistry is available in both the public and the private sector, with both displaying demands for M.Sc Chemistry graduates. MSc Chemistry promises huge career scope to candidates. After completing the course, candidates can work as professionals in Pharmaceutical Companies, Laboratories,

Research Centers, Medical Colleges, private clinics, etc. and also opt for the teaching profession as a professor or a teacher

Mentioned below are some of the sectors which offers potential employability to M.Sc Chemistry graduates

- Academic Institutions
- Pharmaceutical Industry
- Chemical Firms
- Research Centers
- Public Relations

Some of the employability potentials for M.Sc. Chemistry graduates are listed below: after completing MSc Chemistry,

- Students can take teaching jobs at Universities or Sr. colleges by clearing SET or NET-LS examinations.
- Students can take teaching jobs at Jr. Colleges, Kendriya Vidyalaya, Navodaya Vidyalaya, High Schools after completing B.Ed. or respective eligibility criteria.
- Students can do Ph.D. at IIT, NIT, IISER, IISc, BARC, TIFR, Universities, Colleges by clearing NET-JRF, GATE or PET examinations.
- Students can do Ph.D. from foreign Universities, students may get scholarships.
- Students can get jobs as Jr. Scientists, Sr. Scientists, Technicians at BARC, Mumbai
- Research Scientists in various Public Sector Units like ONGC, IOCL, NTPC and Private sector industries.
- Students can become Content Developer for IT industries.
- Students can become Quality Control Chemists/ Food Inspector at Food Co-operation of India, Food Safety and Standards etc
- Student can become Drug Inspector
- Officer at Geological Survey of India
- Laboratory technicians to look after sophisticated instruments like NMR, Mass Spectrometer, UV-Visible Spectrophotometer, Single crystal machines, XRD, SEM, AAS, TEM etc
- Technician for repairing sophisticated instruments
- Lab Technologist/ Lab Chemist
- Synthetic Lab Scientist: Many industries and startups have come up in the recent times to cater the need of R & D and production. These industries hire skilled chemists with a lucrative package.
- Solid State Chemistry Expert : Students skilled in crystallography are hired by the organo- electronics and semiconductor producing industries
- Chemistry/Biochemistry Research Officer : in R& D units of industries
- Analytical Chemistry Application Specialist in industry
- Chemists at Medical colleges, pathologies
- Research Scientist/ Operations Manager/ Chemists / Quality Manager / Research Manager at various industries like Pharmaceuticals, Cement, Plastic, Drugs, Paint, Dyes, Agricultural sector etc
- Student can become Small or medium scale entrepreneur (own industry)
- Students can become Government officers by clearing UPSC, MPSC, Bank Probationary officers, other competitive examinations
- Employee at Security Printing and Minting co-operation of India
- Employee at Office of Controller general of Patent design and trade work
- Free-lancer as educational you tube videos maker
- Educational-aid maker
- Free-lancer for creating awareness about superstition eradication
- Free-lancer to create awareness among farmers about soil testing, pesticides uses etc
- Students can work as come up with NGOs for superstition eradication.

Government jobs:

There are a variety of career prospects waiting to be tapped at the government level. Because there is also a wide scope of research. Some of the government positions that can be considered are-

- Senior Research Associate
- Laboratory Technologist
- Research Analyst
- Research Officer
- Warehouse Supervisor
- Chemists
- Assistant Professor
- Development Supervisor
- Quality Management Analyst

Future Outlook and Scope:

- If the candidates do not wish to pursue job opportunities after M.Sc Chemistry, they can opt for higher education to polish their skills and gain a higher level of experience. They can went on to pursue PhD at premier institutes in India and abroad. They can appear for various competitive exams like NET/ GATE (in India) and JRE/ TOEFEL (Abroad) and avail fellowship for PhD. A significant amount of fellowship is available for pursuing PhD.
- 2. Candidates can acquire education in management and then can join industry or can start their own business or industry.

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| | | | | - | | | | | | ear Sen | nester- I L | evel 6.0 | | | | | | | |
|----------|--|----------------------------|----------------------------|--|-------------------------|--------|----------|-----------------|---|----------------------|------------------------------|--------------------|----------------------------|------------------|--------------|----------------|-------------------|-------------------|-------|
| S. N. | Subject | Type of Course | Subject Code | | Te | aching | g & Lear | ning Scl | heme | | Duration Of Exam Hours | | | Examiı | nation & Eva | aluation Sc | heme | | |
| | | Course | | | | | | | | | nours | | I | Maximum Marks | | | Min | imum Passi | ng |
| | | | | | ching Period Week | Per | | | Credits | | | The | ory | | ctical | Total Marks | | | |
| | | | | L | Т | Р | Total | L/T | Practical | Total | RAK | Theory Internal | Theory +MCQ External | Internal | External | | Marks Internal | Marks External | Grade |
| 0 | *Pre-Requisite Course(s) if applicable/MOOC/Internship/FieldWork cumulatively If students wish to opt Minor Course ofUG as Major for PG, balance 12 Credits Course will have to be completed (As and when applicable) | Th-Prq | | 0 | 0 | 0 | SANT | earnee Credi | tional Credi d = (1) minu its from Maj rses in UG (1 e Credits all from the C nor at UG, n ed as Major | s(2) (1). jorDSC | 2 | 15 | 35 | | | 50 | 06 | 14 | P |
| 1 | Research Methodology and IPR in Chemistry | Th-Major | CHE 100 | 4 | | | 4 | 4 | | 4 | 3 | 30 | 70 | | | 100 | 12 | 28 | Р |
| 2 | DSC-I.1 (Structural Inorganic Chemistry) | Th-Major | CHE 101 | 4 | | | 4 | 4 | | 4 | 3 | 30 | 70 | | | 100 | 12 | 28 | Р |
| 3 | DSC-II.1 (General Organic Chemistry) | Th-Major | CHE 102 | 3 | | | 3 | 3 | | 3 | 3 | 30 | 70 | 3 | | 100 | 12 | 28 | Р |
| 4 | DSC-III.1 (Physical Chemistry-I) | Th- Major | CHE 103 | 3 | | | 3 | 3 | | 3 | 3 | 30 | 70 | | | 100 | 12 | 28 | Р |
| 5 | DSE-I /MOOC (Inorganic/Organic/Physical/ Analytical/Industrial Chemistry) | Th-Major Elective | CHE 104 (i/ii/iii/iv/v) | 4 | | | 4 | 4 | A 1 | 4 | 3 | 30 | 70 | | | 100 | 12 | 28 | Р |
| | | | | | | | 2 | | | | | 3 | 1 | | | | Minimu Mរ | n Passing Irks | Grade |
| 6 | DSC-II.1 Lab (Organic Chemistry Lab) | Pr-Major | CHE 105 | | | 4 | 4 | 1 | 2 | 2 | 4 | 104 | | 50 | 50 | 100 | 5 | 50 | Р |
| 7 | DSC-III.1 Lab (Physical Chemistry Lab) | Pr-Major | CHE 106 | | | 4 | 4 | | 2 | 2 | 4 | | | 50 | 50 | 100 | 5 | 50 | Р |
| 8 | # On Job Training, Internship/ Apprenticeship; Field projects Related to Major @ during vacations cumulatively | Related to DSC | | 120 H cumulative vacations of and Sem | ely dur f Semes | ster I | | | | 4* | | | | | | | | | P* |
| 9 | Co-curricular Courses: Health and wellness, Yoga Education, Sports and Fitness, Cultural Activities, NSS/NCC,Fine/Applied/Visual/Performing Arts During Semester I, II, III and IV | Generic Optional | | 90 H Cumul From Sem I | atively | | | | | | | | | | | | | | |
| | TOTAL | | | | | | | | | 22 | | | | | | 700 | 1 | | |

L: Lecture, T: Tutorial, P: Practical/Practicum

Pre-requisite Course mandatory if applicable: **Prq**, Theory : **Th**, Practical/Practicum: **Pr**, Faculty Specific Core: **FSC**, Discipline Specific Elective: **DSE**, Laboratory: **Lab**, **OJT**: On Job Training: Internship/ Apprenticeship; Field projects: **FP**; **RM**: Research Methodology; Research Project: **RP**, **Co-curricular Courses: CC**

Note : # On Job Training, Internship/ Apprenticeship; Field projects Related to Major (During vacations of Semester I and Semester II) for duration of 120 hours mandatory to all the students, to be completed during vacations of Semester I and/or II. This will carry 4 Credits for learning of 120 hours. Its credits and grades will be reflected in Semester II credit grade report.

Note: **Co-curricular Courses:** In addition to the above, CC also include but not limited to Academic activities like paper presentations in conferences, Aavishkar, start-ups, Hackathon, Quiz competitions, Article published, Participation in Summer school/ Winter School / Short term course, Scientific Surveys, Societal Surveys, Field Visits, Study tours, Industrial Visits, online/offline Courses on Yoga (Yoga for Ego development, Yoga for Ego development, Y



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| | | | <u>(100 100</u> | 5 100 | i sei | lester | | | | | mester- II | Level 6.01 | | <u> </u> | | | | | |
|----------|---|----------------------|----------------------------|----------------------|---|----------------------|--------------|----------|-----------|---------------|------------------------------|------------------------------------|----------------------------|------------|---------------|----------------|-------------------|-------------------|---------|
| S. N. | Subject | Type of Course | Subject Code | | | Teachi | ng & Lear | | | | Duration Of Exam Hours | | | | n & Evaluatio | on Scheme | | | |
| | | | | | | | | | | | nours | | Max | ximum Mark | S | | Min | imum Passin | 5 |
| | | | | ſ | eachin Per | ig Perio Week | d | | Credits | | | The | eory | Prac | tical | Total Marks |] | | |
| | | | | L | Т | Р | Total | L/T | Practical | Total | ken | Theory Internal | Theory +MCQ External | Internal | External | | Marks Internal | Marks External | Grade |
| 1 | DSC-I.2 (Physical Chemistry-II) | Th-Major | CHE 201 | 4 | | 0 | 4 | 4 | | 4 | 3 | 30 | 70 | | | 100 | 12 | 28 | Р |
| 2 | DSC-II.2 (Coordination Chemistry) | Th-Major | CHE 202 | 3 | | 9 | 3 | 3 | 4 Care | 3 | 3 | 30 | 70 | | | 100 | 12 | 28 | Р |
| 3 | DSC-III.2 (Basic Analytical Chemistry) | Th-Major | CHE 203 | 3 | | 3 | 3 | 3 | 1 | 3 | 3 | 30 | 70 | | | 100 | 12 | 28 | Р |
| 4 | DSE-II/MOOC ((Inorganic/Organic/Physical/ Analytical/Industrial Chemistry) | Th-Major Elective | CHE 204 (i/ii/iii/iv/v) | 4 | | | 4 | 4 | - | 4 | 3 | 30 | 70 | | | 100 | 12 | 28 | Р |
| | | | | | | | 4 | | As | A | | 2 | 5 | | | | Minimun Marks | n Passing | |
| 5 | DSC-I.2 Lab (Inorganic Chemistry Lab) | Pr-Major | CHE 205 | | | 4 | 4 | | 2 | 2 | 3 | | | 50 | 50 | 100 | | 50 | Р |
| 6 | DSC-II.2 Lab (Analytical Chemistry Lab) | Pr-Major | CHE 206 | | | 4 | 4 | | 2 | 2 | 3 | 81 | | 50 | 50 | 100 | | 50 | Р |
| 7 | # On Job Training, Internship/ Apprenticeship; Field projects Related to Major @ during vacations cumulatively | Related to Major | | cur durir of S | 20 Hou nulativ 1g vaca Semeste Semest | ely tions er I | | 500 | 119 | 4* | Sec. | 18 | 7 | | | | | | Р* |
| 8 | Co-curricular Courses: Health and wellness, Yoga Education, Sports and Fitness, Cultural Activities, NSS/NCC,Fine/Applied/Visual/Performing Arts, During Semester I, II, III and IV | Generic Optional | | Cu Fro | 0 Hour mulativ m Sem Sem IV | ely I to | 0 | N | | | 33 | 150 | | | | | | | |
| | | | | Exit O _l | Stu | dent ha | is to earn T | Fotal mi | | dits cumul | atively during | p in the respect Vacations of S | | | from interns | hip in orde | er to exit afte | r First Year v | vith PG |
| | TOTAL | | | | | | | | | 18+4* = 22 | | | | | | 600 | | | |

L: Lecture, T: Tutorial, P: Practical/Practicum

Pre-requisite Course mandatory if applicable: **Prq**, Theory : **Th**, Practical/Practicum: **Pr**, Faculty Specific Core: **FSC**, Discipline Specific Core: **DSE**, Laboratory: **Lab**, **OJT**: On Job Training: Internship/ Apprenticeship; Field projects: **FP**; **RM**: Research Methodology; Research Project: **RP**, **Co-curricular Courses: CC**

Note :# On Job Training, Internship/ Apprenticeship; Field projects Related to Major (During vacations of Semester I and Semester II) for duration of 120 hours mandatory to all the students, to be completed during vacations of Semester I and/or II.

This will carry 4 Credits for learning of 120 hours. Its credits and grades will be reflected in Semester II credit grade report.

Note: Co-curricular Courses: In addition to the above, CC also include but not limited to Academic activities like paper presentations in conferences, Aavishkar, start-ups, Hackathon, Quiz competitions, Article published, Participation in Summer school/ Winter School / Short term course, Scientific Surveys, Societal Surveys, Field Visits, Study tours, Industrial Visits, online/offline Courses on Yoga (Yoga for IQ development, Yoga for Ego development, Yoga for Eyesight Improvement, Yoga for Physical Stamina, Yoga for Stress Management, etc.). These can be completed cumulatively during Semester I, II, III and IV. Its credits and grades will be reflected in semester IV credit grade report.



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|--|
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| (Two Years- Four Semesters Master's Degree Programme- NEPv23 with Exit and Entry Option |

| | | | | | | | | N | 1.Sc. (Che | mistry) | Second Ye | ar Semester | r- III [Leve | el 6.5] | | | | | |
|----------|---|----------------------|----------------------------|---|----------------------------------|----------------|------------|----------|-------------------|---------|------------------------------|--------------------|----------------------------|-----------|--------------|----------------|-------------------|-------------------|-------|
| S. N. | Subject | Type of Course | Subject Code | | Т | eaching | g & Learni | ing Sche | eme | | Duration Of Exam Hours | | | Examinat | tion & Evalu | ation Sch | eme | | |
| | | | | | | | | | | | Hours | | Maxi | mum Marks | 5 | | Mir | nimum Pass | ing |
| | | | | Т | eaching Per W | Period 'eek | | | Credits | | ALC: NO | Theo | ory | Pra | ctical | Total Marks | - | | 8 |
| | | | | L | Т | Р | Total | L/T | Practical | Total | our cap | Theory Internal | Theory+ MCQ External | Internal | External | | Marks Internal | Marks External | Grade |
| 1 | DSC-I.3 | Th-Major | CHE 301 | 4 | | | 4 | 4 | 3 | 4 | 3 | 30 | 70 | | | 100 | 12 | 28 | Р |
| 2 | DSC-II.3 | Th-Major | CHE 302 | 4 | | | 4 | 4 | 1 4 | 4 | 3 | 30 | 70 | | | 100 | 12 | 28 | Р |
| 2 | DSC-III.3 | Th-Major | CHE 303 | 3 | | | 3 | 3 | | 3 | 3 | 30 | 70 | | | 100 | 12 | 28 | Р |
| 3 | DSE-III /MOOC (Inorganic/Organic/Physical/ Analytical/Industrial Chemistry) | Th-Major Elective | CHE 304 (i/ii/iii/iv/v) | 3 | | | 3 | 3 | | 3 | 3 | 30 | 70 | | | 100 | 12 | 28 | Р |
| | | | | | | | | | | Ps. | | | 2 | | | | Minimu Ma | m Passing arks | |
| 4 | DSC-III.3 Lab (based on DSC I.3, II.3 and III.3) | Pr-Major | CHE 305 | | | 6 | 6 | 2 | 3 | 3 | 6 | | F/4 | 50 | 50 | 100 | 5 | 50 | Р |
| 5 | DSE-Lab | | CHE 306 | | | 4 | 4 | 1 | 2 | 2 | 6 | 2 | 10 | 50 | 50 | 100 | 5 | 50 | |
| 6 | Research Project Phase-I | Major | | | 2 | 4 | 6 | 2 | 2 | 4 | 3 | 18 | 135 | 50 | | 50 | 2 | 25 | Р |
| 7 | Co-curricular Courses: Health and wellness, Yoga Education, Sports and Fitness, Cultural Activities, NSS/NCC, Fine/Applied/Visual/Performing Arts During Semester I, II, III and IV | Generic Optional | | | Hours ulatively 1 I to Sei | m IV | | N | No. | 5 | AN | 10 | 8 | | | | | | |
| | TOTAL | | | | | | | | | 23 | | | | | | 650 | | | |

L: Lecture, T: Tutorial, P: Practical/Practicum

Pre-requisite Course mandatory if applicable: Prq, Theory : Th, Practical/Practicum: Pr, Faculty Specific Core: FSC, Discipline Specific Core: DSC, Discipline Specific Elective: DSE, Laboratory: Lab, OJT: On Job Training: Internship/ Apprenticeship; Field projects: FP; RM: Research Methodology; Research Project: RP, Co-curricular Courses: CC

Note: Co-curricular Courses: In addition to the above, CC also include but not limited to Academic activities like paper presentations in conferences, Aavishkar, start-ups, Hackathon, Quiz competitions, Article published, Participation in Summer school/ Winter School / Short term course, Scientific Surveys, Societal Surveys, Field Visits, Study tours, Industrial Visits, online/offline Courses on Yoga for IQ development, Yoga for Ego development, Yoga for E

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| | | | | | | | | Ι | 1.Sc. (Ch | emistry |) Second Y | ear Semest | er- III [Lev | | | | | | |
|----------|---|----------------------|----------------------------|----|---|---------------------------------|------------|---------|------------------|---------|------------------------------|-----------------------|----------------------------|-----------|--------------|----------------|-------------------|-------------------|-------|
| S. N. | Subject | Type of Course | Subject Code | | | Te | aching & L | earning | Scheme | | Duration Of Exam Hours | | | Examinat | tion & Evalu | ation Sche | me | | |
| | | | | | | | | | | | nours | | Maxi | mum Marks | 5 | | Mir | nimum Passi | ing |
| | | | | | | iching Period Per Week | | | Credit s | 18A | AMRA | The | ory | | ctical | Total Marks | | | |
| | | | | L | Т | Р | Total | L/T | Practic al | Total | 10 A | Theory Internal | Theory+ MCQ External | Internal | External | | Marks Internal | Marks External | Grade |
| 1 | DSC-I.4 | Th-Major | CHE 401 | 4 | | | 4 | 4 | 10.3 | 4 | 3 | 30 | 70 | | | 100 | 12 | 28 | Р |
| 2 | DSC-II.4 | Th-Major | CHE 402 | 4 | | | 4 | 4 | | 4 | 3 | 30 | 70 | | | 100 | 12 | 28 | Р |
| 3 | DSC- III.4 | Th-Major | CHE 403 | 4 | | | 4 | 4 | | 4 | 3 | 30 | 70 | | | 100 | 12 | 28 | Р |
| 4 | DSE-IV /MOOC (Inorganic/Organic/Physical/ Analytical/Industrial Chemistry) | Th-Major Elective | CHE 404 (i/ii/iii/iv/v) | 3 | | | 3 | 3 | _ | 3 | 3 | 30 | 70 | | | 100 | 12 | 28 | Р |
| | | | | | | | | | | 1/2 | 1 | - | 2 H | | | | Minir Passing | | |
| 5 | DSC- Laboratory (based on I.4, and III.4) | | CHE 405 | | | 2 | 2 | 3 | 2 | 2 | 3 | | 15 11 | 50 | 50 | 100 | 5 | 50 | Р |
| 6 | Research Project Phase-II | Major | CHE 406 | | 2 | 8 | 10 | 2 | 4 | 6 | 3 | 1 | 1 3 2 | 75 | 75 | 150 | 7 | /5 | Р |
| 7 | Co-curricular Courses: Health and wellness, Yoga Education, Sports and Fitness, Cultural Activities, NSS/NCC, Fine/Applied/Visual/Performing Arts During Semester I, II, III and IV | Generic Optional | | Fr | 90 Hours Cumula tively om Sem Sem IV | a I to | 100 | 100 | State of the | | | and the | J. | | | | | | |
| | TOTAL | | | | | | | | | 23 | | and the second second | | | | 650 | | | |

L: Lecture, T: Tutorial, P: Practical/Practicum

Pre-requisite Course mandatory if applicable: Prq, Theory : Th, Practical/Practicum: Pr, Faculty Specific Core: FSC, Discipline Specific Core: DSC, Discipline Specific Elective: DSE, Laboratory: Lab, OJT: On Job Training: Internship/ Apprenticeship; Field projects: FP; RM: Research Methodology; Research Project: RP, Co-curricular Courses: CC

Note: Co-curricular Courses: In addition to the above, CC also include but not limited to Academic activities like paper presentations in conferences, Aavishkar, start-ups, Hackathon, Quiz competitions, Article published, Participation in Summer school/ Winter School / Short term course, Scientific Surveys, Societal Surveys, Field Visits, Study tours, Industrial Visits, online/offline Courses on Yoga (Yoga for IQ development, Yoga for Ego development, Yoga for Anger Management, Yoga for Eyesight Improvement, Yoga for Physical Stamina, Yoga for Stress Management, etc.). These can be completed cumulatively during Semester I, II, III and IV. Its credits and grades will be reflected in semester IV credit grade report.

 Table: Comprehensive Credits distribution amongst the type of Courses over Two Years (Four Semesters) PG Programme and Minimum Credits to be earned for PG Degree

 [M.Sc. (Chemistry)]

| Sr. No. | Type of Course | e | 2 3 | Total Credits Offered | Minimum Credits Required |
|------------|---|----|-------|---|--|
| 1 | MAJOR | | 1 1 | | |
| | i. DSC | 56 | 0 5 | | 56 |
| | ii. DSE | 16 | 5 3 | | 16 |
| | | | TOTAL | 72 | 72 |
| 2 | Research Methodology and IPR (FSC/DSC: Major) | 04 | Se a | 04 | 04 |
| 2 | On Job Training, Internship/ Apprenticeship; Field projects Related to Major | 04 | 23 | 04 for 120 Hours OJT/FP cum. | 02 (Minimum 60 Hours OJT/FP is mandatory) |
| 3 | Research Project | 10 | | 10 | 10 |
| | OPTIONAL | | 2.3 | | 115 |
| 4 | Co-Curricular Courses (offline and/or online as applicable): Co-curricular Courses: Health and wellness, Yoga Education, Sports and Fitness, Cultural Activities, NSS/NCC, Fine/Applied/Visual/Performing Arts, CC also include but not limited to Academic activities like paper presentations in conferences, Aavishkar, start-ups, Hackathon, Quiz competitions, Article published, Participation in Summer school/ Winter School / Short term course, Scientific Surveys, Societal Surveys, Field Visits, Study tours, Industrial Visits, online/offline Courses on Yoga (Yoga for IQ development, Yoga for Ego development, Yoga for Anger Management, Yoga for Eyesight Improvement, Yoga for Physical Stamina, Yoga for Stress Management, etc.). | | | Limited to Maximum 03 only (For 90 Hours of CC cumulatively) | 00 |
| | TOTAL | | | | |
| | TOTAL | | | 93 | 88 |

Table A: Comprehensive Credit Distribution for CC

| 5. N. | Activities (offline/online as applicable) | Credits a | t Levels | | | | | Letter Grade |
|----------|---|-----------|------------|--------|---------------|----------|---------------------------|----------------------|
| N. | | College | University | State | Zone if exist | National | International if exist | 1100 |
| | Health and wellness, Yoga* Competitions *If a Course (online/offline) on Yoga is completed for 60 Hours, 2 credits will be awarded to the student (1 Credit = 30 Hours) | 1 | 2 | 3 | 4 | 5 | 6 | P (Pass) |
| | Unnat Bharat Abhiyan [UBA] | 1 | 2 | 3 | 4 | 5 | 6 | P (Pass) |
| | Sports and fitness activities (see separate Table B) | 1 | 1 / 2 | 2/3 | 3 / 4 | 4 / 5 | 5/6 | P (Pass) |
| ŀ | Cultural activities, Fine/Applied/Visual/Performing Arts | 1 | 2 | 3 | 4 | 5 | 6 | P (Pass) |
| i | N.S.S. activities Camps | 1 | 2 | 3 | 4 | 5 | 6 | P (Pass) |
|) | Academic activities like Research Paper/Article/Poster presentations, Aavishkar, start-up, Hackathon, Quiz competitions, other curricular, co-curricular activities, students exchange programme etc. Research Paper/Article published | 1 | 2 | 3 2 | 4 | 5 | 6 | P (Pass) P (Pass) |
| | Participation in Summer school/ Winter School / Short term course | 2 Credits | | | Q | T | - | P (Pass) |
| | (not less than 30 hours 1 or 2 weeks duration) (not less than 60 hours 2 or 3 weeks duration) | 4 Credits | | | | | | P (Pass) |
| | Scientific Surveys, Societal Surveys | 2 Credit | S | | | | | P (Pass) |
| | Field Visits, Study tours, Industrial Visits, | 1 Credit | | | | | | P (Pass) |
| 3 | NCC Activities | As given | in Table C | | | | | / |

Table B: Credit Distribution for Sports and Fitness

| Sr. | Particulars of Sports Status (Individual/ Team) | Credits | Letter |
|-----|---|---------|----------|
| No. | | | Grade |
| 1 | College Level Participation | 1 | P (Pass) |
| 2 | University Level Participation | 1 | P (Pass) |
| 3 | University Level Rank 1, 2, 3 | 2 | P (Pass) |
| 4 | State Level Participation | 2 | P (Pass) |
| 5 | State Level Rank 1, 2, 3 | 3 | P (Pass) |
| 6 | Zonal Level Participation | 3 | P (Pass) |
| 7 | Zonal Level Rank 1, 2, 3 | 4 | P (Pass) |
| 8 | National Level Participation | 4 | P (Pass) |
| 9 | National Level Rank 1, 2, 3 | 5 | P (Pass) |
| 10 | International Level Participation | 5 | P (Pass) |
| 11 | International Level 1,2,3 | 6 | P (Pass) |

Table C: Credit Distribution for NCC activities

| Sr. No. | Particulars of NCC Activities | Credits | Letter Grade |
|---------|-----------------------------------|---------|-----------------|
| 1 | Participation in NCC activities | 1 | P (Pass) |
| 2 | 'B' Certificate obtained | 2 | P (Pass) |
| 3 | 'C' Certificate obtained | 3 | P (Pass) |
| 4 | State Level Participation | 4 | P (Pass) |
| 5 | National level Participation | 5 | P (Pass) |
| 6 | International Level Participation | 6 | P (Pass) |

Part B

Sant Gadge Baba Amravati University, Amravati Prescribed for (Two Years- Four Semesters Master's Degree Programme- NEPv23 Programme: MSc (Chemistry) following Three Years UG Programme wef 2023-24 Scheme for Teaching, Learning, Examination and Evaluation for M.Sc. Part-I (Chemistry) Semester I

| Subject | Teaching hours per | Credits | Theory | Exam | Practica | al Exam | Total | | mum sing |
|------------------------------------|-----------------------|---------|--------------|--------------|--------------|--------------|-------|--------------|--------------|
| | week | | Intern al | Exter nal | Intern al | Exter nal | | Intern al | Exter nal |
| Research Methodology and IPR | 04 | 04 | 30 | 70 | | | 100 | 12 | 28 |
| DSC – I.1 | 04 | 04 | 30 | 70 | | | 100 | 12 | 28 |
| DSC – II.1 | 03 | 03 | 30 | 70 | | | 100 | 12 | 28 |
| DSC – III.1 | 03 | 03 | 30 | 70 | | | 100 | 12 | 28 |
| DSE - I (i/ii/iii/iv/v) | 04 | 04 | 30 | 70 | | | 100 | 12 | 28 |
| LAB - I | 04 | 02 | | | 50 | 50 | 100 | 5 | 0 |
| LAB - II | 04 | 02 | | | 50 | 50 | 100 | 5 | 0 |
| Total | 26 | 22 | | | | | 700 | | |

| Subject | Course Code | Course Title | Hrs/ | Credits |
|---------------------------------|----------------------|--|------|---------|
| | | | week | |
| Research Methodology and IPR | CHE 100 | Research Methodology and IPR in Chemistry | 4 | 4 |
| DSC – I.1 | CHE 101 | Structural Inorganic Chemistry | 4 | 4 |
| DSC – II.1 | CHE 102 | General Organic Chemistry | 3 | 3 |
| DSC – III.1 | CHE 103 | Physical Chemistry-I | 3 | 3 |
| DSE - I (i) | CHE 104 (i) | Bioinorganic Chemistry | 4 | 4 |
| DSE - I (ii) | CHE 104 (ii) | Organic Reaction Mechanisms | 4 | 4 |
| DSE - I (iii) | CHE 104 (iii) | Polymer Chemistry | 4 | 4 |
| DSE - I (iv) | CHE 104 (iv) | Optical Methods of Analysis | 4 | 4 |
| DSE - I (v) | CHE 104 (v) | Heat Transfer and Mass Transfer | 4 | 4 |
| Lab - I | CHE 105 | Organic Chemistry Laboratory (Lab 01) | 4 | 2 |
| (based on DSC II.1) | | | | |
| Lab - II | CHE 106 | Physical Chemistry Laboratory (Lab 02) | 4 | 2 |
| (based on DSC III.1) | | | | |

| Subject | Teaching hours per | Credits | Theory | / Exam | Practical Exam | | Total | Minimum Passing | |
|-----------------------------|-----------------------|---------|--------------|--------------|----------------|--------------|-------|--------------------|--------------|
| | week | | Intern al | Exter nal | Intern al | Exter nal | | Intern al | Exter nal |
| DSC – I.2 | 04 | 04 | 30 | 70 | | | 100 | 12 | 28 |
| DSC – II.2 | 03 | 03 | 30 | 70 | | | 100 | 12 | 28 |
| DSC – III.2 | 03 | 03 | 30 | 70 | | | 100 | 12 | 28 |
| DSE - II (i/ii/iii/iv/v) | 04 | 04 | 30 | 70 | | | 100 | 12 | 28 |
| LAB - III | 04 | 02 | | | 50 | 50 | 100 | 5 | 0 |
| LAB - IV | 04 | 02 | | | 50 | 50 | 100 | 5 | 0 |
| Total | 22 | 18 | | | | | 600 | | |

M.Sc. Part-I (Chemistry) Semester II

| Subject | Course Code | Course Title | Hrs/ | Credits |
|----------------------|---------------|---|------|---------|
| | | | week | |
| DSC – I.2 | CHE 201 | Physical Chemistry-II | 4 | 4 |
| DSC – II.2 | CHE 202 | Coordination Chemistry | 3 | 3 |
| DSC – III.2 | CHE 203 | Basic Analytical Chemistry | 3 | 3 |
| DSE - II (i) | CHE 204 (i) | Photo-inorganic chemistry and | 4 | 4 |
| | | Organometallics | | |
| DSE - II (ii) | CHE 204 (ii) | Advanced Organic Chemistry | 4 | 4 |
| DSE - I I(iii) | CHE 204 (iii) | Electrochemical Processes and Applications | 4 | 4 |
| DSE - II (iv) | CHE 204 (iv) | Thermal and Electro-Analytical Techniques | 4 | 4 |
| DSE - II (v) | CHE 204 (v) | Unit Processes and Green Chemistry | 4 | 4 |
| Lab - III | CHE 205 | Inorganic Chemistry Laboratory (Lab 03) | 4 | 2 |
| (based on DSC II.2) | | | | |
| Lab - IV | CHE 206 | Analytical Chemistry Laboratory (Lab 04) | 4 | 2 |
| (based on DSC III.2) | | | | |

M.Sc. (Chemistry) First Year Semester- I [Level 6.0]

| Code of the Course/ Subject | Title of the Course/Subject | (Total Number of Periods) |
|--------------------------------|---|------------------------------|
| CHE 100 | Research Methodology and IPR in Chemsitry (FSC) | 60 hrs (4 hrs/week) |

Course Outcomes: At the end of the course, students will be able to

- 1. Formulate research problem
- 2. Test the research hypothesis, understand the data collection and prepare the scientific research paper.
- 3. Identify various meta data sources for literature survey
- 4. Communicate research effectively using various online tools
- 5. Explore on various IPR components and patent writing
- 6. Apply electronic spreadsheets for chemical calculations, data visualization, and plotting.
- 7. Apply probability theorem and probability curves in statistical analysis.
- 8. Perform tests for rejection of data, including T-test, F-test, and Q-test.
- 9. Utilize the least squares method for deriving calibration graphs in chemical analysis.

Unit-I: Introduction to Research (10 hrs)

Definition of research, Characteristics of research, Types of research-Descriptive vs. Analytical, Applied vs. Fundamental, Quantitative vs. Qualitative, Conceptual vs. Empirical. Overview of research methodologies in chemistry, Formulating research questions and objectives. Experimental design and hypothesis formulation,

Unit-II: Literature survey and Scientific Writing and Communication (10 hrs)

Literature survey: Literature review and critical analysis of scientific literature, sources of literature (Print and web), Internet resources for chemistry. Introduction to indexing and citation databases, Research metrics and meta-data, Impact factor, H-index, UGC CARE List of journals, E-books, Google Scholar, Science Direct, Sci-Finder, Scopus.

Scientific Writing and Communication Publishing thesis/project/research paper: Identification of research problem, Survey of literature, Formulation of hypothesis, experimental design and methodology, Analysis of data and interpretation of results, discussion and conclusion, acknowledgements, citations, and referencing. Structure and components of research papers, maintain literature data using software or web resources (Mendeley, EndNote, Zotero)

Unit III: Research and Publication Ethics (10 hrs)

Philosophy and Ethics : Introduction to philosophy and its relevance to research ethics. Ethical principles and moral philosophy in research

Responsible Conduct of Research: Intellectual honesty and integrity in scientific research. Research misconduct: Falsification, fabrication, and plagiarism. Selective reporting and misrepresentation of data

Publication Ethics : Introduction to publication ethics and its importance. Best practices and standards in publication ethics (e.g., COPE, WAME). Conflicts of interest in research publication. Authorship and contributorship guidelines. Identification and handling of

publication misconduct. Predatory publishers and journals. Introduction to plagiarism detection software (e.g., Turnitin, Urkund) Ethical issues.

Unit-IV: IPR: : Basic concept of Intellectual Property, Rationale behind Intellectual Property, intellectual property rights and patent law in India. Structure and Components of Indian patents Types of IP: Patents, Designs, Trademark, Copyright, technological research, innovation, Techniques of writing a patent.

Unit-V: Data collection and analysis

(10 hrs)

Data, types of data and sources of data. Data curation. Introduction to electronic spreadsheets and their functionalities, Application of Electronic Spreadsheets in Chemistry, Data analysis and visualization techniques using spreadsheets in chemistry, Spreadsheet applications for chemical calculations, data management, and plotting. Interpretation of research data.

Collection, Treatment and presentation of analytical data. True, standard and observed value. Definition of terms in mean and median. Errors in chemical analysis, classification of errors, nature and origin of errors.

Unit-VI: Statistical Analysis: (Emphasis should be placed on numerical problems) (10 hrs)

Accuracy and precision. Average deviation and standard deviation and its physical significance. Normal distribution curve and its properties. Coefficient of variation. Confidence limit and probability. Probability theorem, probability curves, comparison of analytical results. Tests for rejection of data. T-test, F-test and Q-test. Significant figures and computation rules. Least squares method for deriving calibration graph. Chemometrics: brief introduction and Statistical approaches for chemists.

Course Material/Learning Resources

- Research Methodology a step-by-step guide for beginners. Ranjit Kumar, SAGE Publications, 3rd Edition, 2011
- 2. Guide to Publishing a Scientific paper, Ann M. Korner, Bioscript Press 2004.
- 3. Intellectual Property Rights Under WTO, T. Ramappa, S. Chand, 2008
- 4. Property Rights, Law and Practice, The Institute of Company Secretaries of India, Statutory Body Under an Act of Parliament, September 2013.
- 5. Research Methodology: Methods and Techniques, C.R. Kothari, Gaurav Garg, New Age International, 4th edition, 2018.
- 6. Research Methods: the concise knowledge base, Trochim, Atomic Dog Publishing, 2005.
- 7. Conducting Research Literature Reviews: From the Internetto Paper, FinkA, Sage Publications, 2009.
- 8. Research methodology: an introduction for science & engineering students, Stuart Melville and Wayne Goddard, Juta & Company, 1996.
- 9. "Philosophy of Science" by A. Bird
- 10. "A Short History of Ethics" by A. MacIntyre
- 11. "On Being a Scientist: A Guide to Responsible Conduct in Research" by National Academy of Sciences, National Academy of Engineering, and Institute of Medicine
- 12. P. Chaddah, "Ethics in Competitive Research: Do Not Get Scooped, Do Not Get Plagiarized"
- 13. D.B. Resnik, "What is Ethics in Research and Why It Is Important?"
- 14. J. Beall, "Predatory Publishers are Corrupting Open Access"
- 15. "Ethics in Science Education, Research and Governance" by Indian National Science Academy (INSA)
- 16. Intellectual Property in New Technological Age, Robert P. Merges, Peter S. Menell and Mark A. Lemley, Aspen Publishers, 2016.
- 17. Resisting Intellectual Property, Halbert, Taylor & Francis Ltd, 2007.
- 18. Industrial Design, Mayall, McGraw Hill, 1992.
- 19. Product Design, Niebel, McGraw Hill, 1974.
- 20. Introduction to Design, Asimov, Prentice Hall, 1962.

Web resources:

- 1. https://onlinecourses.nptel.ac.in/noc22_ge08/preview
- 2. <u>https://www.youtube.com/watch?v=_Mb_cNqfsdc</u>
- 3. <u>https://www.youtube.com/watch?v=hHHPGLqz6zo</u>
- 4. Academic Integrity and Research Quality by the University Grants Commission, https://www.ugc.gov.in/e-book/Academic%20and%20Research%20Book WEB.pdf
- 5. UGC Guidance Document: Good Academic Research Practices, <u>https://www.ugc.gov.in/e-book/UGC GARP 2020 Good%20Academic%20Research%20Practices.pdf</u>

M.Sc. (Chemistry) First Year Semester- I [Level 6.0]

| Code of the Course/ Subject | Title of the Course/Subject | (Total Number of Periods) |
|--------------------------------|--|------------------------------|
| CHE 101 | Structural Inorganic Chemistry (DSC–I.1) | 60 hrs (4 hrs/week) |

Course Outcomes: At the end of the course, students will be able to:

- 1. predict the nature of bond and its properties through various electronic structural methods; bonding models
- 2. recognize and assign symmetry characteristics to molecules and objects,
- 3. understand and analyze structure-property correlation of carbonyls, clusters boron hydrides
- 4. design new metal carbonyls based on a fundamental understanding of their electronic properties
- 5. calculate EAN of carbonyls and nitrosyls.
- 6. appreciate specialized and advanced topics in inorganic and coordination chemistry
- 7. corelate structure and bonding with reactivity of boron clusters

UNIT I: VSEPR Theory

Postulate of VSEPR theory, Recap of shapes of regular geometries. Predicting types of hybridization of central atom in a molecules/ions (shape or geometry and bond angles) (with and without lone pair of electrons) like SbF₄⁻, SF₅⁻, SeF₃⁻, ICl₂⁻, ICl₄⁻, IF₄⁻, IOF₄⁻, NH₂⁻, NH₄⁺, I₃⁻, PCl₂⁺, PCl₆⁻, SO 4²⁻, ClF₃, IF₆⁻, BrF₅, XeOF₄, XeF₄, XeO₃, SOF₂, IF₅, [BF₄]⁻, [I 5]⁺, [Br₃]⁺, BCl₃,SnF₃, XeF₂O₂,ClO₃⁻, [TeF₅]⁻, [BeF₄]⁻, [SbCl₆]³⁻, [PF₆]⁻ etc.; Advantages and disadvantages (Drawbacks) of VSEPR theory, Bent's rule.

UNIT II: Molecular Orbital Theory & Hypervalents

A) Postulates of molecular orbital theory, molecular orbital representation of polyatomic molecules with special reference to CH₄, NH₃, H₂O, PF₅, SF₆, B₂H₆ and CO and delocalised molecular orbital of ozone, carbon dioxide, nitrite, nitrate and benzene.

B) Hypervalent (expanded octet) inorganic species/molecules/ions/compounds, Iso-structural and iso-electronic pair/species/ions: General idea with examples

UNIT III: Symmetry and group theory

10 hrs

18

10 hrs

10 hrs

Symmetry elements and symmetry operations: Rotational axis of symmetry and types of rotational axes, plane of symmetry and types of planes, improper rotational axis of symmetry, inversion centre and identity element; more about symmetry elements; Symmetry operation as matrices; Molecular point groups: Definition and notation of point groups, Classification of molecules in to C₁, C_s, C_i, Cn,C_nv, C_nh, C_∞v, D_n, D_nh, Dnd, D_{∞h}, Sn(n=even), T_d, O_h, I_h groups; Group multiplication table for C_{2v} & C_{3v}, reducible and irreducible representation, great orthogonality theorem (without proof) and its importance, construction of character table of C_{2v} & C_{3v} point group.

UNIT IV: Boron Cage compounds

A) Boron Hydride: IUPAC nomenclature, classification (closo, nido, arachno and klado), structure, bonding and topology of boranes, 4-digit coding (STYX rule and/or Lipsocomb rule) numbers for B₂H₆, B₃H 8, B₃H 9, B₄H₁₀, B₅H 9, B₅H₁₁, B₆H₁₀, B₆H₁₂, B₇H₁₁, B₈H₁₂, B₁₂H₁₄ etc, polyhedral skeletal electron pair theory (WADE'S rule), Bronsted acidity of higher boranes.

B) Carboranes and Metallocarboranes: Classifications, nomenclatures, types, cage and

geometry according to WADE'S rule.

UNIT V: Metal carbonyl and nitrosyls

A) Metal Carbonyl: Basic ideas (18 electron counting rule, hapticity, ligand contribution to electron counting including CO as a ligand), classification, preparation and uses of metal carbonyls, EAN rule, MO's of CO; nature of bonding in metal carbonyls, modes of ligation (bonding modes) by CO as a ligand (Terminal and bridging) bond order of CO and IR spectroscopy, Carbonyl clusters, types of carbonyl clusters, calculation of number of M-M bonds by WADES rule of metal carbonyl cluster.

B) Metal nitrosyls: Types, preparation and properties, Structure and use of sodium nitroprusside, structure and nature of metal-nitrosyl bond in metal nitrosyla, EAN rule

UNIT VI: Non-Carbonyl metal cluster:

10 hrs

10 hrs

General idea of multiple metal-metal bonds, Quadruple bonding in di and/or binuclear cluster (including MO diagrams, bond order, structure, symmetry, conformation and electronic transition selection rule) Ex: $[Mo_2Cl_8]^{4-}$, $[Mo_2(SO_4)_4]^{4-}$, $[Os_2Cl_8]^{2-}$, $[Re_2Cl_9]^-$ and $[Re_2Cl_8]^{2-}$ [Re2(Me₂PPh)₄Cl₄), $[Re_2Cl_4(PMe_2Ph)_4]^+$, $[(Bu_4N)_2Re_2Cl_8], [W_2(OPh)_6]$, $[W (CH_3)_8]^{4-}$ etc, Preparation, properties and structures (A/C to Wades rules) of Zintl (Naked cluster) anions & cation of the metal Ge, Sn, Pb, Sb, Bi.

Course Material/Learning Resources

- 1. Selected Topics In Inorganic Chemistry: W.U. Malik, G.D. Tuli & R.D. Madan (S. Chand Publications)
- 2. Symmetry and Spectroscopy of Molecules: K Veera Reddy New Age International publishers, 2014.
- 3. Group Theory and its Chemical Applications P.K. Bhattacharya (Himalaya Publishing House) 2003
- 4. Concise Coordination Chemistry : R Gopalan and V Ramalingam (Vikas publishing House Pvt Ltd)
- 5. B.R. Puri, L.R Sharma and K.C. Kalia, Principles of Inorganic Chemistry, Vishal publication, 2016
- 6. Advanced Inorganic Chemistry Volume I Satya Prakash, G.D. Tuli, S K Basu& R.D. Madan (S. Chand Publications)
- 7. Advanced Inorganic Chemistry Volume II Satya Prakash, G.D. Tuli, S K Basu& R.D. Madan (S. Chand Publications)
- 8. Symmetry and Group theory in Chemistry, Mark Ladd, Marwood Publishers, London (2000).
- 9. Molecular Symmetry and Group Theory, Robert L.Carter, John Wiley & Son (1998).
- 10. Inorganic Chemistry, 5th Edition: Gary L. Miessler, Paul J. Fischer and Donald A. Tarr Pearson Publication.
- 11. Advanced Inorganic Chemistry. F.A.Cotton, G.Wilkinson, C.A.Murillo and M.Bochmann, 6th Edition, Wiley Interscience, N.Y (1999

10 hrs

- 12. Inorganic Chemistry, J.E. Huheey, K.A.Keiter and R.L.Keiter 4 th Edition Harper Cottens College Publications (1993).
- 13. Inorganic Chemistry, Keith F.Purcell and John C.Kotz, Holt-Saunders International Editions, London (1977).
- 14. Advanced Inorganic Chemistry 3rd, 5th & 6th Editions.: F.A. Cotton& G. Wilkinson:
- 15. Theoretical Approach in inorganic chemistry: A.F. Willims
- 16. Atomic Structure and chemical Bonding: Mannas Chanda

Web resources:

- 1. Basics of Inorganic Chemistry https://nptel.ac.in/courses/104101121
- 2. VSEPR- https://nptel.ac.in/courses/104101090
- 3. Symmetery and Group Theory:<u>https://onlinecourses.nptel.ac.in/noc22_cy40/preview</u>
- 4. Ligational Aspects of Diatomic molecules- https://nptel.ac.in/courses/104106064

| M.Sc. | (Chemistry) | First Year S | Semester- | I [Level 6 | .0] |
|-------|-------------|--------------|-----------|-------------|-----|
| | | | | | |

| Code of the Course/ Subject | Title of the Course/Subject | (Total Number of Periods) |
|--------------------------------|--|------------------------------|
| CHE 102 | General Organic Chemistry (DSC–II.1) | 60 hrs (4 hrs/week) |

Course Outcomes: At the end of the course, students will be able to:

- 1. Implement rules of aromaticity to organic molecules
- 2. Evaluate the organic reactions based on the influence of the substituents on substrate molecules
- 3. Design organic reactions based on free radical chemistry in order to achieve the required product(s)
- 4. Sketch organic molecules in different projection formula and assign its configuration.
- 5. Compare the stability of different conformers
- 6. Apply their understanding about the organic reactions of industrial significance with respect to the chemo- selectivity, regioselectivity and enantioselectivity.
- 7. Analyze the product distribution and the stereochemistry of various organic products.

Unit I Electronic effects and Aromaticity:

(7 Hrs)

(7 Hrs)

Delocalized chemical bonding, conjugation, cross conjugation, resonance, hyper-conjugation, inductive Resonance effects. Aromaticity in benzenoid and non-benzenoid compounds, alternant and non-alternant hydrocarbons Huckel's rule, energy level of π -molecules orbitals, annulenes, antiaromaticity, homo-aromaticity. quasi-aromatic compound, Aromatic character and chemistry of cyclopentadienyl anion, Systems of Two Electrons (cyclopropenyl cation), tropylium cation, tropone and tropolone, Frost Circles (The Polygon Method) for drawing energy levels in cyclic pi systems.

Unit II Reaction Intermediates: Carbene and Nitrene

Carbene: Types of carbenes, Structure and reactivity of carbenes, Generation, structure and reactions, insertion, addition, rearrangement reactions of carbenes, nucleophilic attack on carbenes, Simmons-Smith reaction, ReimerTiemann reaction, Carbylamine reaction, **Nitrene**: Generation, structure and reactions

Unit III Free radical chemistry and name reaction:

Introduction of free radical, generation types, structure and stability of free radical reactions, free radical initiator (heat/light/benzoyl or dibenzoyl peroxide/AIBN) and abstracting reagents (Tributyl tin hydride/triphenyl tinhydride/trimethyl silyl hydride/NBS/SmI2). Hunsdiecker reaction, allylic and benzylic bromination (Wohl-Ziegler), methane and vinylic bromination (using NBS), Sandmeyer, Fentons reagents and its applications. The Bergman cyclization reaction, chlorosulphonation (Reed Reaction).

Unit IV Free radical rearrangement, coupling reaction and application. (8 Hrs)

A) Photo-fragmentation/rearrangements reactions: Barton-nitrite reaction, hypohalite reaction, Barton McCombie deoxygenation reaction, Barton-radical decarboxylation reaction, Hoffmann-Loeffler Freytag reaction.

B) Free radical coupling reactions: i) Ullman reaction, ii) McMurry coupling reaction, iii) Pinacol type coupling reaction.

C) Applications of tributyltin hydride (TBTH): i) Dehalogenation followed by intramolecular radical addition to carbon-carbon double and triple bonds, Tandem or Cascade radical cyclization, ii) Inter and intramolecular dehalogenation (Reduction of halides), iii) Reduction of carbonyl to alcohols, iv) opening of the cyclopropane and epoxide ring

Unit V Basic Stereochemistry:

Isomerism, Concept of chirality and molecular dissymmetry Enantiomeric relationships, diastereomeric relationships, Cahn-Ingold-Prelog System to describe configuration at chiral centers R and S, E and Z nomenclature, molecules with more than one chiral center, meso compounds, threo and erythro isomers, Homotopic, Enantiotopic, and Diastereotopic Groups (Faces), method of resolution, optical purity, topicity of ligands, prochirality, Inter conversion of Newman, Sawhorse and Fischer projection.

Unit VI Advanced Stereochemistry:

Introduction of optical activity in the absence of chiral carbon (biphenyls, spiranes, allenes and helical structures). Chirality in Substituted adamantane, Chirality of heteroatoms, Conformational analysis of cycloalkanes (5-8 membered rings), substituted cyclohexanes (mono, di and tri), decalin system, effect of conformation on reactivity, Conformational analysis of n-butane and its derivatives, ethylene glycol, 1,2-dihaloethane and related compounds.

Course Material/Learning Resources

- 1. J. March and M. B. Smith, March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 6th Edition, Wiley, 2013.
- 2. Jagdamba Singh's Organic Chemistry Concepts & Applications (Pragati Prakashan)
- 3. D. Nasipuri, Stereochemistry of Organic Compounds Principles and Applications, New Age International Publishers, 3rd Edition, 2011
- 4. Peter Sykes, A Guidebook to Mechanism in Organic Chemistry, 6th Edition, Pearson Education Ltd., England, 2013
- 5. J. Clayden, N. Greeves, S. Warren and P. Wothers, Organic Chemistry, 1st edition, Oxford University Press, 2001
- 6. Free Radical in Organic Chemistry Jacques Fossey, Daniel Lefort & Jannie Sorba Willey Publication.
- 7. Radical Reactions in Organic Synthesis Samir Z.Zard. Oxford Chemistry Masters.
- 8. Stereochemistry of Organic Compounds: Ernast Eliel Willey Publication
- 9. Stereochemistry of Organic Compounds: V K Ahluwalia Springer Publication
- 10. K. Peter C. Vollhardt and N. E. Schore, Organic Chemistry, W. H. Freeman and Company 1999

(8 Hrs)

(8 Hrs)

(7 Hrs)

- 11. Organic Chemsitry as a Second Language: David R Klein, Jon Wiley and Sons, 2004
- 12. L. Finar, Organic Chemistry Vol. I & Vol. II, Longman (Cambridge), 2011.
- 13. F. A. Carey and R. J. Sundberg, Advanced Organic Chemistry Part B: Reaction and Synthesis, Springer, 5th Edition, 2010.
- 14. Organic Chemistry (7th edition) : R.T. Morrison and R.N. Boyd. Pearson Publication

Web resources :

- 1. Introductory Organic Chemistry I- https://nptel.ac.in/courses/104106119
- 2. Radical Chain Polymerization-<u>https://www.youtube.com/watch?v=RwmXApb_KXk</u>
- 3. Stereochemistry- https://nptel.ac.in/courses/104105086
- 4. Stereochemistry and Applications- https://nptel.ac.in/courses/104106127
- 5. Structure, Stereochemistry and Reactivity of Organic Compounds and Intermediates: A Problem solving Approach-<u>https://nptel.ac.in/courses/104105127</u>
- 6. Stereochemistry: https://chem.ucr.edu/sites/default/files/2019-10/Chapter4.pdf

| Code of the Course/ Subject | Title of the Course/Subject | (Total Number of Periods) |
|--------------------------------|--|------------------------------|
| CHE 103 | Physical Chemistry - I (DSC–III.1) | 60 hrs (4 hrs/week) |

Course Outcomes: At the end of the course students will be able to

- 1. Understand basic and advanced level statistical thermodynamics, and reaction kinetics, electrolytic conductance
- 2. Apply the concepts of statistical thermodynamics and reaction kinetics to solve complex problems.
- 3. Demonstrate the ability to use chemical dynamics to solve problems associated with enzyme kinetics, and complex reactions
- 4. Implement and build theoretical models for reaction rates, thermodynamics, conductometric and potentiometric titration
- 5. Solve numerical problems associated with statistical thermodynamics, reaction kinetics.

Unit-I: Kinetics of Complex Reactions

Kinetics of Complex Reactions: Chain reaction (H₂+Br₂, \rightarrow 2HBr thermal and photo chemical reaction), Homogeneous catalysis (acid-base and enzymes), oscillating reactions (BelousovZhabotinsky reaction, Lotka-Volterra mechanism, the brusselator and the oregonator).

Enzyme Kinetics: Michaelis-Menten kinetics, Multi-substrate reactions, Lineweaver-Burk plot

Unit-II: Theories of Reaction Rates

Theories of reaction rates: Collision theory, collision rates in gases, energy requirement and steric requirement. Dynamics of molecular collisions. Transition state theory: assumptions, Statistical Mechanics and Chemical equilibrium, derivations of Eyring equation, Application of transition state theory to reaction between atoms and molecules (e.g. The reaction $H + HBr \rightarrow H_2+Br$)

Unit-III: Fast reactions and Theory of Unimolecular Reactions

A) Fast reactions: General Features and examples of fast reactions, Stopped flow method, Rlaxation method, Nuclear Magnetic Resonance method, Flash Photolysis, Numerical.

B) Theory of Unimolecular reactions: Lindemann-Christiansen hypothesis and Hinshelwood treatment, Marcus's extension of the RRK treatment

Unit-IV: Electrochemistry

Electrochemistry: Strong electrolyte , weak electrolyte and molar conductivity, Debye Huckle theory of conductance, Ionic atmosphere, relaxation effect, Electrophoretic effect ,Debye Huckel Onsagar equation, validity and deviation of the Debye Huckel Onsagar equation, ionic strength, activity and activity coefficient of strong electrolyte, Debye Huckle limiting law, Derivation and modification of Debye Huckle limiting Law, numerical.

8 Hrs

7 Hrs

8Hrs

7 Hrs

Unit-V: Statistical Thermodynamics

Statistical entropy, microcanonical and canonical ensembles. Ideal monoatomic and diatomic gases Thermodynamic probability, most probable distribution. Maxwell-Boltzmann distribution law Fermi-Dirac statistics, distribution law and applications to metals. Bose-Einstein statistics-distribution law and application to helium. Applications of statistical thermodynamics to activated complex theory

Unit-VI: Partition functions

7 Hrs

Partition function: Translational, rotational, vibrational and electronic partition functions, calculations of thermodynamic properties in terms of partition functions. Applications of partition functions. Numerical.

Course Material/Learning Resources

Text books:

- 1. McQuarrie, D. A.; Simon, J. D.; Physical Chemistry: A Molecular Approach, University Science Books, 2011.
- 2. Atkins, P. W.; Paula, J.; Physical Chemistry, Oxford Publications, 11th edition.
- 3. McQuarrie, D. A.; Statistical mechanics, University Science Publishers, 2000

Reference Books:

- 1. Hill, T. A.; an Introduction to Statistical Thermodynamics, Dover Publications Inc., 1987.
- 2. Levine, I. N.; Physical Chemistry, McGraw-Hill Science/Engineering/Math, 6th edition, 2008.
- 3. Laidler, K. J.; Chemical Kinetics, Pearson Education, 3rd edition, 2011
- 4. Physical Chemistry R.A. Alberty, R.I. Bilby, Johy Wiley 1995
- 5. Physical Chemistry G.M. Barrow, Tata Mc Graw Hill 1988
- 6. Statistical thermodynamics, by T.L.Hill, Addison Wesley, 1060 Chemical thermodynamics, by F.T. Wall, W.H.Freeman & Co. 1965
- 7. Irreversible thermodynamics, Theory and applications, by K.S.Forland, T. Forland, S.KRatje, Jonny Witey, 1988.
- 8. Chemical Kinetics, by K. J. Laidler, 3rd Edition, Harper and row, 1987.
- 9. Chemical Kinetics-A study of reaction rate in solution, K.Conors, V.C.H.Publkatkm 1990.
- 10. Chemical Kinetics and Dynamics, By J.I.Streinfeld, J.S. Francisco & W.I.Hase, Pritice Hall, 1989.
- 11. Kinetics and Mechanism of Chemical transformation, J.Rajraman, J. Kucriacose, Mc-Million
- 12. Molecular reaction Dynamics and chemical reactivity, R.D.Levine and R.B. Benstin, Oxford University ress. 1987.
- 13. Physical Chemistry by Alberty and Silby, Jolly Wiley.

Web resources:

Approximate Methods In Quantum Chemistry: <u>https://nptel.ac.in/courses/104105128</u> Advanced Chemical Thermodynamics and Kinetics: <u>https://nptel.ac.in/courses/104106094</u> Thermodynamics: Classical to statistical: <u>https://nptel.ac.in/courses/104103112</u> 8 Hrs

| M.Sc. (Chemistry) First Year Sem | ester- I Level 6.0 |
|----------------------------------|----------------------|
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| Code of the Course/ Subject | Title of the Course/Subject | (Total Number of Periods) |
|--------------------------------|-------------------------------|------------------------------|
| CHE 104 (i) | Bioinorganic Chemistry | 60 hrs |
| | (DSE–I (i)) | (4 hrs/week) |

Course Outcomes: At the end of the course, students will be able to:

- 1. Describe the principles and concepts of bio-inorganic chemistry, including the role of inorganic elements and compounds in biological systems.
- 2. Describe the coordination chemistry of metal ions in biological processes, such as metalloenzymes, metalloproteins, and metallocofactors.
- 3. Explain the biochemical processes involving essential inorganic elements, including their transport, uptake, and metabolism in living organisms.
- 4. Analyze the electronic structure, bonding, and spectroscopic properties of metal complexes in biological systems.
- 5. Analyze the interplay between bio-inorganic chemistry and other areas of chemistry and biology, such as bioorganic chemistry, medicinal chemistry, and environmental chemistry.
- 6. Apply the principles of chelate therapy to propose rational solutions and approaches for addressing biological and biomedical challenges, such as drug design, metal toxicity, and biomaterials development.

Unit-I: Essential trace elements in biological systems

Perspective of essential trace elements viz V, Cr, Mn, Fe, Co, Cu & Zn and their influence of excess and deficiency, regulation and storage of trace elements, genetic defects in the absorption of trace elements; Coordination by proteins, tetrapyrrole ligands and other macrocycle and biomineralization with respect to ferritin, transferrin and siderophores; Role of calcium in transport and regulation in living cells; Vanadium storage and transport.

Unit II: Transport & Storage of Dioxygen and electron

- A) Transport & Storage of Dioxygen: Heme proteins & oxygen uptake, structure and functions of haemoglobin, myoglobin, hemocyanins & hemerythrin. Perutz mechanism showing structural changes in porphyrin ring system. Oxygenation and deoxygenation. Model compounds. Cyanide poisoning and treatment.
- **B)** Transport of Electrons: Iron-Sulphur Proteins: Rubredoxins and Ferredoxins (2Fe, 3Fe, 4Fe, 8Fe Proteins) High Potential Iron-Sulphur Proteins –Structural and Spectral features of Iron-Sulphur Proteins Electron-transport by Cytochromes, Azurin and Plastocyanin -Importance of Structures of Azurin and Plastocyanin in facilitating Rapid Electron Transport.

Unit III: Transport and Storage of Metal Ions, Bio-energetics and ATP cycle:

- A) Transport and Storage of Metal Ions: Iron-Transport by Transferrin and Siderophores-Ferritin in Iron Storage - Transport of Na⁺ and K⁺ across Cell Membranes by Na⁺, K⁺ ATPase-Transport of Calciumacross Sarcoplasmic Reticulam by Ca²⁺ATPase.
- **B)** Bio-energetics and ATP cycle: DNA polymerization, metal complexes in transmission of energy, chlorophylls, photosystem-I and photosystem-II in cleavage of water.

Unit IV: Chelate therapy:

10 hrs

A brief introduction to chelate therapy and its types; Therapeutic spectra of different chelating drugs in metal ion detoxification; Chelating drugs containing sulphydryl group, the polyaminocarboxylic acids, polyethyleneamines, desferrioxamines; Radioprotective chelating drugs, limitations and hazards in chelation therapy;

Unit V: Metallotherapy:

Medicinal use of metal complexes as antibacterial and anticancer; Aanticancer activity of platinum(II) and platinum(IV) complexes, mechanism of the anticancer activity of platinum

10hrs

10hrs

10 hrs

complexes, mode of action of cisplatin; Anticancer activities of rhodium, gold, copper and cobalt complexes. Metal complexes as probes of nucleic acid, metal ions in genetic regulations, metal DNA and RNA interaction – Potential binding sites.

Unit VI: Metalloenzymes:

10 hrs

Apoenzymes, Haloenzyme & Coenzyme; The principle involved and role of various metals enzymes- i) Zn-enzyme: Carboxyl peptidase & Carbonic anhydrase; ii) Fe-enzyme: Catalase Peroxidase & Cytochrome P-450; iii) Cu-enzyme: Super Oxide dismutase; iv) Co-enzyme vitamin B_{12} : Structure, Co-C bond cleavage and mutase activity; Alkylation reactions of methyl cobalamine, synthetic model of enzyme action, stability and ageing of enzyme; v) Nickel Enzyme: Urease, Hydrogenase and factor F430: Reactions catalysed, mechanistic aspects.

Course Material/Learning Resources

- 1. Das A. K.: A Text Book on Medicinal Aspects of Bio-inorganic Chemistry.
- 2. Akhmetov, N.: General and Inorganic Chemistry.
- 3. Aylett, B. and Smith, B.: Problems in Inorganic Chemistry, (English University Press)
- 4. Bertini, et al: Bioinorganic Chemistry (Viva)
- 5. Charlot, G and Bezier, D.: Quantitative Inorganic Analysis (john Wiley).
- 6. Douglas, B. E. Mc Danirl, D. H. et al: Concept and Models of Inorganic Chemistry (4th edt.) J. Wiley
- 7. Dutt P. K.: General and Inorganic Chemistry. (Sarat Books House)
- 8. Fenton, David E.: Bio-coordination chemistry, Oxford
- 9. Jolly, W. L.: Inorganic Chemistry (4th edn.) Addison-Wesley.
- 10. Katakis, D. and Gordon, G.: Mechanism of Inorganic Reactions. (J. Wiley).
- 11. Leigh, G. J.: IUPAC Nomenclature of Inorganic Chemistry (1990; Jain-Interscience)
- 12. Massey, A. G.: Main Group Chemistry.
- 13. Porterfield, W. W.: Inorganic Chemistry-A unified approach (Holt Saunders)
- 14. Banerjee, D.: Coordination Chemistry, TMH
- 15. Lee J. D., Concise Inorganic Chemistry, ELBS
- 16. Lippard S.J and Berg, J. M.: Principal of Bioinorganic Chemistry, University Sci. Book., Mill Valley
- 17. Hay R. W.: Bioinorganic Chemistry, Ellis Horwood, Chichester and NY
- 18. Das A.K.: Text Book of Medicinal Aspects of Bioinorganic Chemistry, CBS
- 19. Sigel H.: Metal ions in Biological systems, Marcell Dekker, NY(Vol.1-31)
- 20. Reddy K.H., Bioinorganic Chemistry, New Age Int. Pub.
- 21. Kaim W. and Schwederski B.: Bioinorganic Chemistry: Inorganic elements in the Chemistry of Life, John Wiley & Sons.
- 22. Medicinal Inorganic Chemistry, Edited by Jonathan L. Sessler, Oxford University Press.

Web resources:

Bioinorganic chemistry - https://nptel.ac.in/courses/104105130

Inorganic Chemistry of Life: Principles and Perspectives-https://nptel.ac.in/courses/104101093

| Code of the Course/ Subject | Title of the Course/Subject | (Total Number of Periods) |
|--------------------------------|---|------------------------------|
| CHE 104 (ii) | Organic Reaction Mechanism (DSE–I (ii)) | 60 hrs (4 hrs/week) |

M.Sc. (Chemistry) First Year Semester- I [Level 6.0]

Course Outcomes: At the end of the course, students will be able to:

- 1. Predict the orientation and stereochemistry of the product of addition reaction
- 2. Apply enolate chemistry to achieve molecular complexity
- 3. Predict the orientation and stereochemistry of the product of elimination reaction
- 4. Justify the formation of products in the reaction due to anchimeric assistance
- 5. Design organic reactions in order to achieve the required product(s).
- 6. Write the reactions and mechanism for the functionalization of aromatic ring

Unit I Addition to C-C multiple bonds:

Mechanistic and stereochemical aspects of addition reaction involving electrophiles, nucleophiles and free radicals, Regio and chemo selectivity, Orientation and stereochemistry, Addition to cyclopropanes, halogenation, hydro-halogenation, hydro-oxy addition, Hydro-alkoxy addition, Hydro-acyloxy addition, hydro alkylthio addition. Alkyl-halo-addition Acyl-halo-addition, hydroboration-oxidation, oxymercuration-demercuration reaction, Michael addition, Baylis-Hillman reactions.

Unit II Addition to carbon-hetero atom multiple bond:

Ionization of carbon hydrogen bond and prototrophy, keto-enol equilibria, structure and rate in enolization, concerted and carbanion mechanism for tautomerism, kinetic and thermodynamic control enolates, Base and acid catalysed halogenation of ketones (Haloform reaction and halogenation on carbonyl). Hydrolysis of esters and amide. Mechanisms and synthetic applications of condensation reactions involving enolates- Aldol,Claisen, Mannich, Knoevenagel Dieckmann Reaction Perkin, Stobbe reaction, Robinson annulation.

Unit III Elimination reaction:

The E1, E2 and E1CB mechanisms. Stereochemistry of E2 elimination. Orientation of the double bond, Saytzeff's and Hoffman's rule, (factors that affect elimination reactions) Effect of substrate structure, attacking base, leaving group and medium, Elimination in cyclohexane systems, Eliminations in bridged compounds—Syn Elimination. Mechanism and orientation in pyrolytic elimination involving Hofmann, selenoxide, Cope and Chagaev elimination.

Unit IV Aliphatic NS and neighbouring group assistance (NGP): (10 Hrs)
 A) Aliphatic nucleophilic substitution (SN): The SN1, SN2, mixed SN1, SN2 and SET and SNi mechanisms. Factors that affect the substitution reaction (Nucleophilicity, effect of leaving group, ambient nucleophiles and ambient substrates regiospecificity), substitution at allylic and vinylic carbon atoms.

B) Neighbouring group assistance (NGP): Anchimeric assistance with mechanism, neighbouring group participation by π and σ bonds, classical and non-classical carbocations,

(10 Hrs)

(10 Hrs)

(10 Hrs)

Intramolecular displacement by hydrogen, oxygen, nitrogen, sulphur and halogen. Alkyl, cycloalkyl, aryl participation, participation in bicyclic system, migratory aptitude.

Unit V Aromatic electrophilic substitution:

(10 Hrs)

The arenium ion mechanism, orientation and reactivity, energy profile diagrams. electrophilic substitution reaction of benzene(halogenation, sulphonation, nitration) The o/p ratio, ipso attack, orientation in benzene ring with more than one substituent, orientation in another ring system. Friedel-Crafts reaction (alkylation and acylation), Vilsmeir-Hack reaction, Gattermann reaction, Gattermann-Koch reaction, Pechman reaction, Diazonium coupling, Blanc chloromethylation, Kolbe–Schmitt reaction.

Unit VI Aromatic Nucleophilic Substitution and Benzyne: (10 Hrs)

A general introduction to different mechanisms of aromatic nucleophilic substitution SNAr, SN1, benzyne and SRN1 mechanisms,

Benzyne: Structure, methods of generations and reactions, arynes as reaction intermediate, Reactivity. Factors that affect the reaction (effect of substrate structure leaving group and attacking nucleophile). The Von Richter and Smiles rearrangements, Chichibabin amination reaction. Benzyne: Structure, methods of generations and reactions.

Course Material/Learning Resources

- 1. March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, J. March and M. B. Smith, 6th Edition, Wiley, 2013
- 2. Organic Synthesis, László Kürti and Barbara Czakó, Elsevier Inc., 2005
- 3. Electrophilic Additions to Carbon-Carbon Multiple Bonds Part B Reactions & Synthesis Francis A. Carey & Richard J. Sundberg (Springer)
- 4. Molecular Rearrangements in Organic Synthesis Christian M. Rojas
- 5. Green Chemstry A Text Book-V.K.Ahluwalia
- 6. Introduction to Green Chemistry- Albert S.Matlack, Second Edition
- 7. J. Clayden, N. Greeves, S. Warren and P. Wothers, Organic Chemistry, 1st edition, Oxford University Press, 2001
- 8. Modern methods of Organic Synthesis W.Carruther&I.Coldham 4th Edition Cambridge
- 9. Modern Organic Synthesis 1st edition by George S. Zweifel, Michael H. Nantz
- 10. Clayden Organic Chemistry (2nd Edition) Solution Manual
- 11. Organic Chemistry (7th edition) : R.T. Morrison and R.N. Boyd. Pearson Publication
- 12. Organic Chemistry by I. L. Finar Vol.I Pearson Publication
- 13. Molecular Orbitals and Organic Chemical Reactions: Student Edition-Ian Fleming Second Edition.

Web Resources:

- 1. Essentials of Oxidation, Reduction and C_C Bond Formation. Application in Organic Synthesishttps://nptel.ac.in/courses/104101127
- 2. Environmental Chemistry-https://nptel.ac.in/courses/105107176
- 3. Principles Of Organic Synthesis-<u>https://nptel.ac.in/courses/104103110</u>
- 4. Introductory Organic Chemistry II-<u>https://onlinecourses.nptel.ac.in/noc21_cy46/preview</u>
- 5. Introduction to Rearrangement Reactions-<u>https://www.youtube.com/watch?v=QhY7tncG_gU</u>
- 6. Wagner-Meerwein rearrangment, Pinacol rearrangment, Benzilic acid rearrangementhttps://www.youtube.com/watch?v=dnam2PHjuwQ
- 7. Rearrangement to electron-Rich carbon-https://www.youtube.com/watch?v=4CjTT5CQ-Jw

M.Sc. (Chemistry) First Year Semester- I [Level 6.0]

| Code of the Course/ Subject | Title of the Course/Subject | (Total Number of Periods) |
|--------------------------------|--|------------------------------|
| CHE 104 (iv) | Optical Methods of Analysis (DSE–I (iv)) | 60 hrs (4 hrs/week) |

Course Outcomes: At the end of the course, students will be able to:

- 1. comprehend of various spectroscopic techniques and their applications in analytical chemistry
- 2. apply Beer's Law and verify its deviations, interpret fluorescence and phosphorescence spectra using Jablonski Diagram, and analyze complex compositions using Job's and mole ratio method
- 3. demonstrate proficiency in operating single and double-beam spectrophotometers, evaluating sensitivity and significance of molar extinction coefficients, and employing derivative spectrophotometry for enhanced spectral analysis
- 4. comprehend the principles and instrumentation involved in atomic absorption, emission, and fluorescence spectrometry, as well as X-ray fluorescence and emission spectroscopy.
- 5. apply optical methods of analysis in various analytical applications.

Unit-I: Spectrophotometry (10h)

- Principles of Spectrophotometry and Colorimetry
- Beer's Law, Verification, and Deviations
- Instrumentation: Single and Double Beam Spectrophotometers
- Sensitivity and Analytical Significance of Molar Extinction Coefficient and λmax
- Quantitative Estimation: Comparison Method, Calibration Curve Method, and Standard Addition Method
- Ringbom Plot and Sandell's Sensitivity
- Photometric Titrations and pK Determination of Indicators
- Simultaneous Determination in Binary Systems
- Complex Composition: Job's and Mole Ratio Methods
- Derivative Spectrophotometry
- Numerical Problems

Unit-II: Fluorimetry and Phosphorimetry (10)

Origin of Fluorescence and Phosphorescence Spectra

- Jablonski Diagram and Electronic Transitions
- Activation and Deactivation Processes
- Fluorescence Spectrum Characteristics

Fluorescent and Phosphorescent Species

- Photoluminescence and Molecular Structure
- Factors Influencing Fluorescence and Phosphorescence

Fluorescence Quenching

- Mechanisms of Quenching
- Quantum Yield Calculation

Instrumentation for Fluorescence Measurement

- Light Sources and Wavelength Selectors
- Sampling Techniques
- Detectors and Readout Devices

Instrumentation for Phosphorescence Measurement

- Sampling Procedures
- Recording Techniques
- Applications of Fluorescence and Phosphorescence
- Analytical Applications
- Biochemical and Biomedical Applications
- Environmental Monitoring
- Material Science and Nanotechnology

Unit-III: Atomic Absorption Spectrometry (10h)

Atomic Absorption Spectroscopy (AAS):

- Principle of AAS and the concept of atomic energy levels
- Understanding Grotrian diagrams and population of energy levels
- Instrumentation involved in AAS analysis
- Sources used in AAS: Hollow cathode lamp and electrodeless discharge lamp, and factors affecting spectral width
- Atomizers used in AAS: Flame atomizers, graphite rod, and graphite furnace
- Cold vapor and hydride generation techniques in AAS
- Factors influencing atomization efficiency and flame profile
- Monochromators and detectors used in AAS analysis
- Beam modulation techniques in AAS
- Detection limit, sensitivity, and considerations for AAS analysis
- Interferences in AAS and methods for interference removal
- Comparison between AAS and flame emission spectrometry
- Applications of AAS in analytical chemistry

Unit-IV: Atomic Emission Spectrometry (10h)

Atomic Emission Spectrometry:

Principle of Atomic Emission Spectrometry

- Overview of atomic emission spectrometry
- Atomic emission spectrometry using plasma sources
- Introduction to different types of plasma sources

Plasma and its Characteristics

- Inductively Coupled Plasma (ICP)
- Direct Current Plasma (DCP)
- Microwave Induced Plasma (MIP)
- Reasons for using argon as the plasma gas *Instrumentation for ICP-AES*
- Sample introduction techniques in ICP-AES
- Monochromators for wavelength selection
- Detectors for signal detection
- Processing and readout devices for data analysis

Types of Instruments for ICP-AES

- Sequential spectrometers
- Simultaneous spectrometers
- Analytical Methodology in ICP-AES
- Qualitative analysis using ICP-AES
- Quantitative analysis using ICP-AES *Interferences in ICP-AES*
- Spectral interferences
- Physical interferences

- Chemical interferences
- Applications of ICP-AES

• Overview of application areas for ICP-AES

Unit-V: Atomic Fluorescence Spectrometry (10h)

Atomic Fluorescence Spectrometry:

Origin of Atomic Fluorescence

- Explanation of atomic fluorescence phenomenon
- Atomic fluorescence spectrum
- Types of atomic fluorescence transitions

Principle of Atomic Fluorescence Spectrometry

- Understanding the relationship between fluorescence intensity and analyte concentration
- Factors influencing fluorescence intensity
- Instrumentation for Atomic Fluorescence Spectrometry
- Overview of AFS instrumentation
- Radiation sources used in AFS
- Atom reservoirs for sample introduction
- Monochromators for wavelength selection
- Detectors for signal detection
- Readout devices for data analysis

Applications of Atomic Fluorescence Spectrometry

- Overview of application areas for AFS
- Interferences in AFS analysis
- Merits and limitations of AFS technique

Unit-VI: X-ray Fluorescence and Emission Spectroscopy (10h)

X-ray Fluorescence Spectroscopy (XRF):

- Principle of XRF spectroscopy
- Instrumentation: Wavelength dispersive XRF and energy dispersive XRF devices
- Sources and detectors used in XRF analysis
- Comparison between wavelength dispersive and energy dispersive techniques
- Sample preparation methods for XRF analysis
- Matrix effects in XRF analysis
- Applications of XRF in qualitative and quantitative analysis
- Particle Induced X-ray Emission (PIXE):
- Basic principle of PIXE
- Instrumentation used in PIXE analysis
- Applications of PIXE in analytical chemistry

Course Material/Learning Resources

- 1. "Principles of Instrumental Analysis" by Douglas A. Skoog, F. James Holler, and Stanley R. Crouch
- 2. "Atomic Absorption Spectrometry" by Bernard L. Sharp
- 3. "Introduction to X-ray Spectrometry" by Ronald Jenkins and Robert L. Snyder
- 4. "Scanning Electron Microscopy and X-ray Microanalysis" by Joseph I. Goldstein, Dale E. Newbury, et al.
- 5. "Analytical Chemistry: Principles and Techniques" by Higson, Barry R.
- 6. "Handbook of X-ray Spectrometry" by Rene Van Grieken and Andrzej Markowicz
- 7. "Atomic Spectroscopy: Introduction to the Theory of Hyperfine Structure" by K. Siegbahn
- 8. "Quantitative Chemical Analysis" by Daniel C. Harris.
- 9. "Analytical Chemistry" by Gary D. Christian.
- 10. "Fundamentals of Analytical Chemistry" by Douglas A. Skoog, Donald M. West, and F. James Holler.

Journals and Publications:

• Analytical Chemistry (American Chemical Society)

- Journal of Analytical Chemistry (Springer)
- Analytica Chimica Acta (Elsevier)
- Talanta (Elsevier)
- Journal of Chromatography A (Elsevier)

Online Databases:

- PubChem: A free database of chemical structures, properties, and biological activities.
- National Institute of Standards and Technology (NIST) Chemistry WebBook: Provides thermophysical and chemical property data for various compounds.
- Royal Society of Chemistry (RSC): Offers a range of analytical chemistry resources, including journals, databases, and books.

Online Courses and Tutorials:

• NPTEL and SWAYAM: Platforms offering online courses and tutorials on analytical chemistry topics.

Analytical Instruments Manufacturers:

• Companies such as Agilent Technologies, Thermo Fisher Scientific, Shimadzu, and PerkinElmer provide resources on their websites, including application notes, webinars, and technical documents.

Academic Institutions:

• University websites often host lecture notes, course materials, and research publications related to analytical chemistry.

Analytical Chemistry Societies:

- American Chemical Society (ACS) Division of Analytical Chemistry: Provides resources and updates on analytical chemistry research and events.
- Royal Society of Chemistry (RSC) Analytical Division: Offers publications, conferences, and networking opportunities.

Online Forums and Communities:

• Chemistry Stack Exchange and ResearchGate: Platforms where scientists and researchers discuss analytical chemistry topics and share knowledge.

| Code of the Course/ Subject | Title of the Course/Subject | (Total Number of Periods) |
|--------------------------------|-------------------------------------|------------------------------|
| CHE 104 (iii) | Polymer Chemistry (DSE–I (iii)) | 60 hrs (4 hrs/week) |

M.Sc. (Chemistry) First Year Semester- I [Level 6.0]

Course Outcomes: At the end of the course, students will be able to:

- 1. Demonstrate a comprehensive understanding of the basic concepts of polymers, including monomers, repeat units, and degree of polymerization.
- 2. Identify and classify different types of polymers based on their structure, composition, and polymerization techniques.
- 3. Apply knowledge of polymer processing techniques to produce plastic, elastomer, and fiber-based products using various processing methods.
- 4. Analyze and interpret the chemical reactions involved in polymerization, including condensation, addition, and copolymerization reactions.
- 5. Utilize different characterization techniques to determine the molecular weight, polydispersity, and other properties of polymers.
- 6. Perform chemical analysis, X-ray diffraction, microscopy, and physical testing to evaluate the properties of polymers.
- 7. Evaluate the degradation mechanisms of polymers and understand the impact of thermal, mechanical, and environmental factors on polymer stability.
- 8. Analyze the structure and properties of polymers, including crystalline morphology, glass transition temperature, and the influence of molecular weight and chemical structure on polymer properties.
- 9. Apply knowledge of polymer composites to design and fabricate materials with enhanced properties

through the incorporation of reinforcement materials.

- 10. Examine the characteristics and applications of specific polymers such as polyethylene, polyvinyl chloride, polyamide, polyester, phenolic resin, epoxy resin, silicone polymer, and electrically conducting polymers.
- 11. Synthesize and apply theoretical concepts to solve numerical problems related to polymer properties, molecular weight, and processing parameters.

Unit-I: Polymers and Polymer Processing

- A) Basic concepts: Monomers, repeat units, degree of polymerization, linear branches, and network polymers. Classification of polymers. Polymerization: condensation, addition, radical chain, ionic and coordination, and copolymerization. Polymerization conditions and polymer reactions, polymerization in homogeneous and heterogeneous systems.
- B) Polymer processing: Plastics, elastomers, and fibers. Compounding, processing techniques: calendaring, die casting, rotational casting, film casting, injection molding, blow molding, extrusion molding, thermoforming, foaming, reinforcing, and fiber spinning.

Unit-II: Molecular weight of polymers

Molecular weight of polymers: Polydispersion, average molecular weight concept. Number, weight, and viscosity average molecular weight. Polydispersity and molecular weight distribution. The practical significance of molecular weight. Measurement of molecular weight. End groups, viscosity, light scattering, osmotic, and ultracentrifugation methods. Numerical problems.

Unit-III: Structure, Analysis and Testing of Polymers

Structure: Morphology and order in crystalline polymers, configuration of polymer chains. Crystal structure of polymers. Morphology of crystalline polymers, strain-induced morphology, crystallization, and melting.

Analysis and testing of polymers: chemical analysis of polymers, X-ray diffraction study, microscopy. Thermal analysis and physical testing: tensile strength, fatigue impact, tear resistance, hardness, and abrasion resistance.

Unit-IV: Properties of Polymers

Properties: Physical properties, crystalline melting point, Tm (melting point) of homogeneous series, effect of chain flexibility and other steric factors. Entropy and heat of fusion, the glass transition temperature, the relation between Tg (glass transition temperature) and Tm. Effect of molecular weight, diluents, chemical structures, chain topology, branching, and cross-linking. Property requirements and polymer utilization. Numerical problems.

Unit-V: Polymer Composites and Functional Polymers

Polymer composites: Polymer matrix materials, reinforcement, properties of composites and composite systems. Fabrication of polymer composites, processing science, and quality assurance of composites, environmental effects on composites, smart composites.

Study of specific polymers: Polyethylene, polyvinyl chloride, polyamide, polyester, phenolic resin, epoxy resin, and silicone polymer. Functional polymer: electrically conducting polymers.

Unit-VI: Polymer Reactions and Degradation

Polymer reactions: Hydrolysis, acetolysis, aminolysis, hydrogenation, addition and substitution reactions, reactions of various specific groups, cyclization reactions, and

10h

10h

10h

10h

10h

10h

cross-linked reactions, reactions leading to graft and block copolymers, miscellaneous reactions.

Polymer degradation: Definition, types of degradation, including thermal, mechanical, degradation by ultrasonic waves, photo degradation, degradation by high-energy radiation, oxidative and hydrolytic degradation.

Text & Reference Books:

- 1. A Textbook of Polymer Science by Billmeyer, Jr. Wiley
- 2. Polymer Science by V.R. Gowarikar, N.V. Vishwanathan & J. Sreedhar, Wiley Eastern.
- 3. Physical Chemistry Polymers by D.D. Deshpande, Tata McGraw Hill.
- 4. Principles of Physical Chemistry by P.J. Flory, Cornell University Press.
- 5. Introduction to Polymer Chemistry by R.B. Seymour, McGraw Hill.
- 6. A Practical Course in Polymer Chemistry by S.J. Pnnea, Program Press.
- 7. Polymer Composites by M.C. Gupta & A.P. Gupta, New Age International Publication.

| M.Sc. (Chemistry) First Year Semester- I [Level 6.0 | M.Sc. | (Chemistry) | First Year Semester- | I [Level 6.0] |
|--|-------|-------------|----------------------|----------------|
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| Code of the Course/ Subject | Title of the Course/Subject | (Total Number of Periods) |
|--------------------------------|---|------------------------------|
| CHE 104 (v) | Heat Transfer and Mass Transfer (DSE–I (v)) | 60 hrs (4 hrs/week) |

Course Outcomes: At the end of the course, students will be able to:

- 1. understand the basics of heat Transfer and Fluid Flow
- 2. find the principle involved in unit operations and their applications in Industry.
- 3. have mechanistic aspects of various Industrial Equipment's.
- established Material balance equation of various unit operations. 4.
- solve material balance equation of mass transfer operations. 5.

Unit I:

A) Fundamentals of Heat transfer: Methods of heat transfer, Fourier s law, Newton s law, heat transfer by conductance, by convection and by radiation. Heat exchanger, types of heat exchanger, overall heat transfer co-efficient, double pipe heat exchanger, Shell & tube type etc.

B) Fluid flow: Fluid flow phenomenon, introduction, Laminar flow, Turbulant flow, Reynolds number, Bernoulli equation, fans, blowers, compressors, pumps etc.

Unit II:

A) Distillation: Introduction, Flash distillation, differential distillation, rectification, plate columns, packed columns, azeotropic distillation

B) Extraction: Introduction, selection of solvent, single stage and multistage extraction, spray column, packed column, mixer settler, Rotating Disc Contactor.

Unit III

A) Leaching: Introduction, Single and Multistage Leaching, Leaching Equipments- Percolation Tank, Countercurrent Multiple Contact (Shank System), Continuous Countercurrent Decantation, Agitated Vessel, Kennedy Extractor.

B) Evaporation: Introduction, Short tube Evaporator, forced circulation evaporator, falling film, Long tube Evaporator, agitated evaporators.

Unit IV

A) Filtration: Introduction, Filter media, filter aids, equipments sparkler filter, sand filters, bag filters, rotary drum filter.

B) Crystallization: Introduction, solubility, super-saturation, nucleation, crystal growth, equipments tank crystallizer, Swenson-Walker crystallizer, Oslo crystallizer.

Unit V:

10 Hrs

10 Hrs

10 Hrs

10 Hr

A) Drying: Introduction, free moisture, bound moisture, Rate of Drying. Equipments: tray dryer, fluid bed dryer, drum dryer, spray dryer, rotary dryer.

Unit VI:

10 Hrs

A) Material Balance Without Chemical Reactions: Material balance without chemical reactions, flow diagram, without recycle or by-pass for above processes. Problems based on above.

B) Material balances involving chemical reactions: Concept of limiting reactant, excess reactant, yield and selectivity, stoichiometric coefficient and stoichiometric equation conversion, purge operation and Problems.

Course Material/Learning Resources:

- 1) Heat transfer By Arora and Damkondwar, Pune
- 2) Heat and Mass transfer by K.A. Gavhane, Nirali Prakashan. Pune VOL I & II.
- 3) Unit operations of Chemical Engineering ,McCabe and Smith, , McGraw Hill.
- 4) Introduction to Chemical Engineering, Budger and Banchero, McGraw Hill.
- 5) Text Book of Industrial Chemistry Pragati Agencies Pune.
- 6) Engineering Chemistry By Dr. S. S. Dara.
- 7) Hand book of industrial chemistry Vol I & II K. H. Davis & F.S. Berner Edited by S.C. Bhatia, CBSpublishers
- 8) Fundamentals of Heat And Mass Transfer" by Incropera F. P.
- 9) Unit Operation -I by K. A. Gavhane.
- 10) Unit Operations" by G. G. Brown.

M.Sc. (Chemistry) First Year Semester- I [Level 6.0]

| Code of the Course/ Subject | Title of the Course/Subject | (Total Number of Periods) |
|--------------------------------|-------------------------------------|------------------------------|
| CHE 105 | Organic Chemistry Laboratory | 60 hrs |
| | (Lab 01) | (4 hrs/week) |
| | (based on DSC-II.1) | |

Course Outcomes: At the end of the course students will be able to

- 1. Design the methodologies to develop ecofriendly and green technology for industry and research.
- 2. Develop methods and remedies for reactions with environmental pollution.
- 3. Improve scientific practical information orally and in writing.
- 4. Get awareness about laboratory safety and handling of chemicals.
- 5. Separate mixture into its constituent using physical and chemical methods of separation.

<u>Part-A</u>

In the beginning of the chemistry practical 4 hrs will be given for

- Laboratory safety: what precautions should be taken while working in chemistry laboratory (working with acids and bases)
- Where to get chemicals information (MSDS)
- Introduction of equipment used for chemistry practical.
- Making apparatus for experiments, correct laboratory techniques.
- Introduction to Use of computer, software's in chemistry, use of OER for virtual practical approach.
- Introduction about Pre lab preparation for every experiment.

<u>Part-B</u>

Organic synthesis will be carried out on reactions involving protection and deprotection, oxidation, reduction, carbon-carbon multiple bonds, Metals/ metal salts catalyzed coupling reactions, Diels-Alder reactions, aromatic substitution reactions, diazotization reactions, condensation reactions, hydrolysis reactions etc.

Organic Preparations (Minimum 8)

- 1. Benzaldehyde to cinnamic acid (Perkin Reaction)
- 2. Diel's Alder reaction of anthracene and maleic anhydride (furan and maleic acid in water).
- 3. p- Chlorotoulene from p-Toluidine. (Sandmeyer reaction)
- 4. Mannich Rection (reaction of primary amine, formaldehyde and carbonyl compound)
- 5. Synthesis of dihydropyrimidinone by Green Method (Biginneli reaction)
- 6. Photoreduction of benzophenone to benzopinacol in the presence of sunlight.
- 7. Synthesis of indigo/Dye and dyeing of cloth
- 8. Synthesis of biodiesel.
- 9. Benzaldehyde to chalcone
- 10. Nitrobenzene to m-di-nitrobenzene
- 11. m-di-nitrobenzene to m-nitroaniline
- 12. Benzoic acid to ethylbenzoate
- 13. Benzyl alcohol and benzoic acid from benzaldehyde (Cannizzaro reaction)
- 14. Benzilic acid from benzoin (Benzilic acid rearrangement)
- 15. Benzopinacol (Photochemical reaction)
- 16. Benzanilide (Beckmann rearrangement
- 17. Phthalic acid \rightarrow Phthalimide \rightarrow Anthranilic acid

Important Note:

- i) The preparations should be carried out using (0.02 to 0.05 mole) of the starting material.
- ii) The yield, melting point and TLC of the recrystallized product should be recorded.
- iii) The sample of the purified product and TLC plate should be submitted for inspection. Draw TLC in the journal and also calculate the Rf value.

iv) Use of Computer - Chem Draw or Chem-Sketch or ISIS–Draw or KingDraw: Draw the structure of product synthesized. Get the correct IUPAC name and interpret of its ¹HNMR as obtained from software.

Part-C

Qualitative Organic Analysis: (Minimum 8 Mixtures)

Separation, purification and identification of binary mixtures by Chemical and physical methods.

The two components may be solid-solid, solid- liquid and liquid-liquid (volatile/nonvolatile). The water soluble solid/liquid should also be given. Student should purify separated compounds from the mixture and prepare a suitable derivative of the two compounds to confirm.

Examination: CHE 105 Organic Chemistry Laboratory (Lab 01)

Time : 6-8 Hrs. (One day Examination)

Total Marks: 100

| А. | Exercise-I (preparation) | 20 |
|----|---|-----|
| В. | Exercise-II (Separation and identification) | 20 |
| C. | Viva (External + Internal) | 10 |
| Е. | Internal assessment* | 50 |
| | Total | 100 |

*- Internal assessment will be continuous and based on the performance of a student throughout the session along with satisfactory submission of the term work

Course Material/Learning Resources:

- 1. Experiments and technique in organic experiments- D. Pasto, C. Johnson and M. Miller prentice Hall.
- 2. Macro- scale and micro-scale organic experiments-K.L. Williaman, D. C. Heath.
- 3. Systematic quantitative organic analysis H. Middleton, Edward Arnold.
- 4. Vogel's Textbook of practical organic chemistry Fifth Edition-Brain S. Furniss, Antoy J. Hannaford, Peter W,G. Smith, Austin R. Tatchell.
- 5. Qualitative organic Chemial analysis-A.I. Vogel.
- 6. Experiment organic chemistry Vol.I&II P.R. Singh, D. S. Gupta and K.S. Bajpai.
- 7. The Golden book of chemistry experiments- Robert Brent

Web resources:

- 1. Detection of functional group: <u>https://vlab.amrita.edu/index.php?sub=2&brch=191&sim=345&cnt=1</u>
- 2. Detection of element: <u>https://vlab.amrita.edu/index.php?sub=2&brch=191&sim=344&cnt=1</u>
- 3. Procedure for synthesis : <u>http://orgsyn.org/Default.aspx</u>

M.Sc. (Chemistry) First Year Semester- I [Level 6.0]

| Code of the Course/ Subject | Title of the Course/Subject | (Total Number of Periods) |
|--------------------------------|-------------------------------|------------------------------|
| CHE 106 | Physical Chemistry Laboratory | 60 hrs |
| | (Lab 02) | (4 hrs/week) |
| | (based on DSC–III.1) | |

Course Outcomes: At the end of the course students will be able to

- 1. Apply knowledge to determine reaction rate of chemical reactions
- 2. Create methods for estimation of concentration of electrolytes in mixture using potentiometry.
- 3. Corelate nature of graphs in conductometric titrations
- 4. Improve skill to perform experiment in electroanalytical methods
- 5. Corelate structure property relationship of conjugated systems
- 6. Design conjugated polymer of desired optoelectronic property.

Part A

- 1. To study the kinetics of Iodine Clock Reaction
- 2. Determine the specific reaction rate of the potassium persulphate-iodide reaction.
- 3. Study the kinetics of the iodination of acetone in the presence of acid.
- 4. Study of enzyme-substrate catalysis reaction: the hydrolysis of p-nitrophenyl phosphate as catalysed by alkaline phosphatase
- 5. Study of an Oscillating Reaction: the oscillating reaction (Belousov-Zhabotinsky) to be studied using the Ce3+/Ce4+ system; dependence of the oscillation period on the metal ion concentration to be monitored.
- 6. Determine the specific rate constant for the acid catalyzed hydrolysis of methyl acetate.
- 7. Study the kinetics of saponification of ethyl acetate with sodium hydroxide volumetrically
- 8. Determine the Critical Micelle Concentration (CMC) of surfactant by surface tension measurements.
- 9. Determine the Critical Micelle Concentration (CMC) of ionic surfactants by conductivity measurements.
- 10. Determination of Critical Micelle Concentration (CMC) and Surface Excess concentration of surfactant using Gibbs adsorption Isotherm
- 11. Ab-initio calculation of rotational barrier between eclipsed and staggered conformation of ethane
- 12. Calculation of potential energy surface of H₂O₂ molecule using HF/6-31G(d,p)
- 13. Particle in 1D Box: Quantum mechanical calculation of HOMO-LUMO gap in ethene, 1,3 butadiene and 1,3,5-hexatriene.

Part B

- 1. To determine equivalent conductance of weak electrolyte at infinite dilution using Kohlrausch law
- 2. Study the conductometric titration of (i) Acetic acid vs. sodium hydroxide, (ii) Acetic acid vs. ammonium hydroxide, (iii) HCl vs. NaOH and comment on the nature of the graphs.
- 3. Titrate a mixture of (i) Strong and weak acids (Hydrochloric and acetic acids), (ii) Weak acid (acetic acid) and dibasic acid (oxalic acid) (iii) Strong acid (hydrochloric acid) and dibasic acid (oxalic acid) versus sodium hydroxide and comment on the nature of the graph
- 4. Study the stepwise neutralization of a polybasic acid e.g. oxalic acid, citric acid, succinic acid by conductometric titration and explain the variation in the plots.
- 5. Titrate conductometrically a moderately strong acid (salicylic/ mandelic acid) by the
 - a. salt-line method
 - b. double alkali method.
- 6. Titrate conductometrically a mixture of copper sulphate, acetic acid and sulphuric acid with sodium hydroxide.
- 7. Titrate conductometrically a tribasic acid (phosphoric acid) against NaOH and Ba(OH)₂ conductometrically.
- 8. Titrate conductometrically magnesium sulphate against BaCl₂ and its reverse titration
- 9. Estimate the concentration of each component of a mixture of AgNO₃ and HNO₃ by conductometric titration against NaOH.
- **10.** Determine the degree of hydrolysis of aniline hydrochloride conductometrically.

- 11. Determine the solubility and solubility product of an insoluble salt, AgX (X=Cl, Br or I) potentiometrically.
- 12. Determine the mean activity coefficient ($\gamma \pm$) of 0.01 M hydrochloric acid solution potentiometrically.
- 13. Study the titration phosphoric acid potentiometrically against sodium hydroxide.
- 14. Find the composition of the zinc ferrocyanide complex by potentiometric titration.
- 15. Determination of thermodynamic constants ΔG, ΔH, ΔS for Zn⁺²+H₂SO₄-→ ZnSO₄+ 2H⁺ by emf measurement
- 16. Titrate potentiometrically solutions of mixture of KCl + KBr + KI and determine the composition of each component in the mixture.
- **17.** Verify the Debye-Hückel theory through the solubility of ionic salts.
- **18.** To determine equivalent conductance of strong electrolyte at several dilution and hence verify Onsagar equation.
- 19. Determine the dissociation constant of acetic acid potentiometrically.

CHE 106 Physical Chemistry (Lab 02)

Time : 6-8 Hrs. (One day Examination)Total Marks : 100

| (1) Exercise-1 (Part A) (2) Exercise 2 (Part P) | 20 Marks 20 Marks |
|---|----------------------|
| (2) Exercise-2 (Part B)(3) Viva-Voce | 20 Marks 10 Marks |
| (4) Internal * | 50 Marks |

Total -100 Marks

*- Internal assessment will be continuous and based on the performance of a student throughout the session along with satisfactory submission of the term work.

Course Material/Learning Resources:

- 1. J. B. Yadav, Practical Physical Chemistry
- 2. Das and Behra, Practical Physical Chemistry
- Carl W. Garland, Joseph W. Nibler and David P. Shoemaker, Experiments in Physical Chemistry, Mc-Graw Hill, 8th Edition, 2009.
- 4. Farrington Daniels, Joseph Howard Mathews, John Warren Williams, Paul Bender, Robert A. Alberty, Experimental Physical Chemistry, Mc-Graw Hill, Fifth Edition, 1956.
- 5. John W. Shriver and Michael George, Experimental Physical Chemistry, Lab Manual and Data Analysis, The University of Alabama in Huntsville, Fall 2006
- 6. Jahgirdar D.V: Experiments In Chemistry

| Code of the Course/ Subject | Title of the Course/Subject | (Total Number of Periods) |
|--------------------------------|----------------------------------|------------------------------|
| CHE 201 | Physical Chemistry-II (DSC–II.2) | 60 hrs |
| | | (4 hrs/week) |

Course Outcomes: At the end of the course students will be able to

- 1. Understand basic concepts and theories for quantum mechanics, surface chemistry, and thermodynamics
- 2. Apply the concepts of quantum mechanics to solve higher order problems associated with shapes, size and energy of atomic entities.
- 3. Develop the methodologies to identify and use colloidal substances and micelles.
- 4. Implement and build theoretical and experimental processes using thermodynamics and electrochemical concepts
- 5. Solve numerical problems associated with quantum mechanics, and thermodynamics.

Unit-I Quantum Mechanics Basics and Simple Systems

- 1. Schrödinger's Equation in One-Dimensional Box (Recapitulation)
 - Review of the time-independent Schrödinger equation for a particle in a one-dimensional box.
 - Energy quantization and wavefunction solutions.
- 2. Postulates of Quantum Mechanics
 - Recapitulation of the fundamental postulates of quantum mechanics.
 - Application of the postulates in various physical systems.
- 3. Hamiltonian Operator
 - General steps involved in construction of Hamiltonian operator for a quantum mechanical system
- 4. Particle in a Three-Dimensional Box
 - Extension of the one-dimensional box to three dimensions.
 - Solution of the Schrödinger equation for a particle in a three-dimensional box.
- 5. Harmonic Oscillator
 - Quantum description of a harmonic oscillator and its energy levels.
 - Wavefunctions and ladder operators.
- 6. Rigid Rotor
 - Quantum treatment of a rigid rotor.
 - Rotational energy levels and wavefunctions.

Unit-II Approximate Methods, Angular Momentum and Electronic Structure of Atoms 10 hrs

- 1. The Variation Theorem and Linear Variation Principle
 - Statement and application of the variation theorem.
 - Linear variation principle and its significance.
- 2. Perturbation Theory (First Order and Non-Degenerate)
 - Introduction to perturbation theory and its application in quantum systems.
 - First-order perturbation theory for non-degenerate energy levels.
- 3. Application to Helium-Like Atom
 - Using variation and perturbation methods to study helium-like atoms.
 - Calculation of energy levels and wavefunctions.
- 4. Ordinary Angular Momentum
 - Properties of ordinary angular momentum and its quantization.
 - Physical significance of angular momentum in quantum systems.
- 5. Generalized Angular Momentum and Eigenfunctions
 - Introduction to generalized angular momentum and ladder operators.

- Calculation of eigenfunctions of angular momentum.
- 6. Pauli Exclusion Principle
 - Statement and implications of the Pauli exclusion principle.
 - Application to multi-electron systems.
- 7. Russell-Saunders Terms and Coupling Schemes
 - Overview of Russell-Saunders terms and coupling schemes in atomic spectra.
 - Determination of term symbols for multi-electron atoms.
- 8. Slater-Condon Parameters
 - Introduction to Slater-Condon parameters and their significance.
 - Calculation of Slater-Condon parameters for atomic systems.

Unit-III Molecular Orbitals and Conjugated Systems

- 1. Construction of Molecular Orbitals by LCAO for H2+ Ion
 - Linear combination of atomic orbitals (LCAO) approach for molecular orbitals.
 - Application to the hydrogen molecular ion (H2+).
 - 2. Energy Levels and Physical Picture of Bonding and Anti-Bonding Wave Functions
 - Calculation of energy levels from molecular wavefunctions.
 - Understanding bonding and anti-bonding orbitals.
- 3. Concept of Orbitals and Their Characteristics
 - Recapitulation of atomic and molecular orbitals.
 - Orbital characteristics and their significance.
- 4. Hybrid Orbitals (sp, sp2, sp3)
 - Introduction to hybridization and its implications.
 - Calculation of hybrid orbital coefficients.
- 5. Huckel Theory of Conjugated Systems
 - Overview of Huckel theory for conjugated systems.
 - Calculation of bond order and charge density.
- 6. Applications to Ethylene, Butadiene, Cyclopropenyl Radical, Cyclobutadiene
 - Applying Huckel theory to various conjugated systems.
 - Calculating properties and characteristics of conjugated molecules.

Unit-IV Surface Chemistry

10 hrs

10 hrs

- A) Adsorption: Freundlich adsorption isotherm, Langmuir adsorption isotherm, Gibbs adsorption isotherm, estimation of surface area (BET equation), surface films on liquids, and catalytic activity at surfaces.
- **B)** Micelles: Surface active agents, classification of surface active agents, micellization, hydrophobic interaction, critical micellar concentration (CMC), factors affecting the CMC of surfactants, counter ion binding to micelles, thermodynamics of micellization-phase separation and mass action models, solubilization, micro emulsion, reverse micelles. Numericals.

Unit-V Chemical Thermodynamics

10 hrs

10 hrs

The first and second law of thermodynamics, Carathéodory's principle and its equivalence to the Kelvin Plank and Clausius statement of the Second law of Thermodynamics, extensive and intensive properties, derivation of thermodynamic equations of state, Maxwell's relations, Third law of thermodynamics, Nernst Heat Theorem, unattainability of absolute zero, calculation of entropy based on third law of thermodynamics, residual entropy and its application.

Unit-VI Classical Thermodynamics and Non equilibrium thermodynamics

Classical Thermodynamics: Partial molar properties. Partial molar free energy, Chemical Potential, Partial molar volume and Partial molar heat content and their significances. Determination of these quantities Concept of fugacity, determination of fugacity, numerical.

Non equilibrium Thermodynamics: Thermodynamic criteria for non-equilibrium states. Entropy production and entropy flow for different irreversible processes (e.g. heat flow, chemical reaction, coupled reactions and electrochemical reactions.) Transformations of the generalized fluxes and forces, phenomenological equations. Microscopic reversibility and Onsager's reciprocity relation, Numerical.

Course Material/Learning Resources

Text books:

- 1. Elementary Quantum Chemistry by F. L. Pilar, Dover Publications, Inc. NY, 1990. 2nd Ed.
- 2. Molecular Quantum Mechanics by P. W. Atkins and R. S. Friedman, 3rd Ed., Oxford Univ. Press, 1997.
- 3. Quantum Chemistry by H Eyring, J Walter, and G E Kimball, John Wiley & Sons 1944
- 4. J.O'M Bockris and A.K.N Reddy, Modern Electrochemistry 2A: Fundamentals of Electrodics, Vol II, 2001.
- 5. D. Skoog and D.West, Principles of Instrumental Analysis, Cengage Learning; 6th edition, 2006

Reference Books:

- 1. Physical Chemistry P.W. Atkin, ELBS fourth edition.
- 2. Physical Chemistry R.A. Alberty, R.I. Bilby, Johy Wiley 1995
- 3. Physical Chemistry G.M. Barrow, Tata Mc Graw Hill 1988
- 4. Quantum Chemistry, I. Levine, Fifth edition, Prentice Hall- 19995. Physical Chemistry Thomas Engel, Philip Reid
- 5. Molecular quantum mechanics, Vol. I & II, P. W. Atkins, Oxford University Press, 1970.
- Statistical thermodynamics, by T.L.Hill, Addison Wesley, 1060 Chemical thermodynamics, by F.T. Wall, W.H.Freeman & Co. 1965
- 7. Irreversible thermodynamics, Theory and applications, by K.S.Forland, T. Forland, S. K Ratje, Jonny Witey, 1988.
- 8. Chemical Kinetics, by K. J. Laidler, 3rd Edition, Harper and row, 1987.
- 9. Chemical Kinetics-A study of reaction rate in solution, K.Conors, V.C.H.Publkatkm 1990.
- Chemical Kinetics and Dynamics, By J.I.Streinfeld, J.S. Francisco & W.I.Hase, Pritice Hall, 1989. Kinetics and Mechanism of Chemical transformation, J.Rajraman, J. Kucriacose, Mc-Million Molecular reaction Dynamics and chemical reactivity, R.D.Levine and R.B. Benstin, Oxford University Press 1987.
- 11. Physical Chemistry by Alberty and Silby, Jolly Wiley
- 12. Quantum Chemistry by Ira N. Levine, Prentice Hall,
- 13. Introduction to Quantum Chemistry by A. K. Chandra, Tata McGraw Hill.
- 14. Atkins, P. W.; Paula, J.; Physical Chemistry, Oxford Publications, 8th edition, 2009
- 15. D.R. Crow, Principles and Applications of Electrochemistry, John Wiley & Sons (New York) 2nd edition, 2001.
- Bard, A. J.; Faulkner, L. R.; Electrochemical Methods: Fundamentals and Applications, Wiley, 2nd edition, 2000.

Web resources:

Quantum Chemistry of Atoms and Molecules: https://nptel.ac.in/courses/104101124

Chemistry and Physics of Surfaces and Interfaces: https://nptel.ac.in/courses/104104130

Introduction to Chemical thermodynamics and kinetics: https://onlinecourses.nptel.ac.in/noc22_cy58/preview

Concepts of Thermodynamics: <u>https://onlinecourses.nptel.ac.in/noc22_me103/preview</u>

Thermodynamics: <u>https://onlinecourses.nptel.ac.in/noc22_me88/preview</u>

| Code of the Course/ Subject | Title of the Course/Subject | (Total Number of Periods) |
|--------------------------------|-----------------------------------|------------------------------|
| CHE 202 | Coordination Chemistry (DSC-II.2) | 45 hrs (3 hrs/week) |

Course Outcomes: At the end of the course, students will be able to:

- 1. recollect the principles of electronic structure, bonding and reactivity of coordination complexes
- 2. understand the concept of synthesis and stability of transition metal organometallic complexes
- 3. develop the possible catalytic pathways leading to desired products
- 4. unravel and interpret the magnetic properties of coordination complexes
- 5. Apply principles of metal-ligand bonding in predicting the electronic and structural properties of complexes.
- 6. Analyze the splitting of d orbitals in different coordination geometries (octahedral, square planar, tetrahedral, square-pyramidal, and trigonal bipyramidal complexes) using crystal field theory, considering the Jahn-Teller distortion and spectrochemical series.
- 7. Evaluate the stability of different oxidation states and ionization energies of transition metal ions based on crystal field effects and variation of lattice energy and heats of hydration.
- 8. Compare and contrast the limitations of crystal field theory with the adjusted crystal field theory (LFT or ACFT) and molecular orbital theory (MOT) to better describe metal-ligand interactions in transition metal complexes.

UNIT I: Metal-ligand bonding:

Crystal field theory: Postulates, splitting of d orbitals in octahedral, square planar, tetrahedral, squarepyramidal and trigonal bipyramidal complexes, Jahn-Teller distortion, spectrochemical series, nephelauxetic series, measurement of CFSE in weak/strong ligand fields, structural consequences of crystal field effects, variation of lattice energy and heats of hydration across 1st row transition metal ions, stabilization of unusual oxidation states and ionization energies, Limitations of crystal field theory.

UNIT II: Molecular orbital theory of metal complexes

Theoretical failure of ionic model of CFT. Experimental evidences in support of metal ligand orbital overlaps. Adjusted crystal field theory (ACFT or LFT), Composition of ligand group orbitals, (SALC principle), molecular orbital energy diagrams of octahedral including both σ and π bonding, molecular orbital energy diagrams of tetrahedral, square-planar complexes including only σ bonding; Comparison of CFT,LFT and MOT.

UNIT III: Electronic spectra

Introduction of electronic spectra of transition metal complexes. Derivation of term symbols for ground and excited states of dⁿ configurations, (L-S coupling and j-j coupling), microstates, Selection rule for ligand-field and charge transfer transitions in metal complexes, Relaxation in Selection rules, Electronic spectra of transition metal complexes of the type[$M(H_2O)_n$]ⁿ⁺ spin free and spin paired ML₆ complexes of other geometries with suitableexamples. Spin forbidden transitions and effect of spin-orbit coupling. Evaluation of Dq , B' and β parameters (Konig method), Numericals. Orgel diagrams (d ¹-d⁹ states) and Tanabe–Sugano diagrams of d² and d⁸ configurations of an octahedral environment.

UNIT IV: Magnetochemistry

Fundamental equations in molecular magnetism, magnetic susceptibility and magnetic moment; diamagnetic and paramagnetic behavior of transition metal complexes of different geometries, factors affecting the magnetic properties, temperature dependence of paramagnetism(TDP) and temperature independent paramagnetism(TIP) of complexes, High spin-low spin crossover. Abnormal magnetic properties, orbital contributions and quenching of orbital angular momentum, spin-orbit coupling, magnetic interactions, ferromagnetism and antiferromagnetism. Anomalous magnetic moments and

44

8 hrs

7 hrs

7 hrs

8 hrs

magnetic exchange coupling. Magnetic properties of polynuclear complexes. Magnetic moment, electronic spectra and structure of tetrahalocobalt(II)complexes.

UNIT V: Reaction Mechanism of Transition Metal complexes-I

8 hrs

7 hrs

Types of substitution reactions in transition metal complexes, attacking reagents electrophilic and nucleophilic, Energy profile diagram with terminology includes substrate, transition state or activated complex, Substitution reactions in octahedral complexes (SN¹ and SN²), lability and inertness, interpretation of lability and inertness of transition metal complexes on the basis of VBT and CFT. Factors affecting the lability of a complex, Kinetics of substitution reactions in octahedral complexes: acid hydrolysis, factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism, direct & indirect evidences in favour of conjugate mechanism, anation reaction, reaction without metal ligand bond cleavage.

UNIT VI : Reaction Mechanism of Transition Metal complexes-II

Substitution reaction in square planer complexes: the trans effect, trans-directing series, cis effect, steric effect, solvent effect, effect of leaving group, effect of charge, effect of nucleophile, effect of temperature. Trans effect theories, uses of trans-effect, mechanism of substitution reactions in Pt(II) complexes. Electron transfer reactions. Types of electron transfer reactions, conditions of electron transfer, and mechanism of one-electron transfer reactions, outer sphere and inner sphere mechanisms, two electron transfer reactions.

Course Material/Learning Resources

- 1. Selected Topics In Inorganic Chemistry: W.U. Malik, G.D. Tuli & R.D. Madan (S. Chand Publications)
- 2. B.R. Puri, L.R Sharma and K.C. Kalia, Principles of Inorganic Chemistry, Vishal publication, 2016
- 3. Advanced Inorganic Chemistry Volume I Satya Prakash, G.D. Tuli, S K Basu& R.D. Madan (S. Chand Publications)
- 4. Advanced Inorganic Chemistry Volume I Satya Prakash, G.D. Tuli, S K Basu& R.D. Madan (S. Chand Publications)
- 5. Organometallic & Bioinorganic Chemistry (4th edition): Ajai Kumar; Aaryush Education
- 6. D.F. Shriver and P.W. Atkins, Inorganic Chemistry, Oxford University Press, 5th Edition, 2010.
- 7. J. D. Lee, Concise Inorganic Chemistry, Oxford University Press, 5th Edition, 2014. Dieter Rehder. Bioinorganic Chemistry: An Introduction, Oxford University Press; 1st Edition, 2014
- 8. D. Rehder, E. Nordlander, Bioinorganic chemistry, Oxford University Press India, 2014.
- 9. Inorganic Chemsitry: Catherine E., Housecroft and Alan G Sharp (5th edition) Pearson publication
- 10. Inorganic Chemistry, 5th Edition: Gary L. Miessler, Paul J. Fischer and Donald A. Tarr Pearson Publication.
- 11. Advanced Inorganic Chemistry. F.A.Cotton, G.Wilkinson, C.A.Murillo and M.Bochmann, 6th Edition, Wiley Interscience, N.Y (1999)
- 12. The Organomettalic Chemistry of the transition metals (7th Edition): Robert H Crabrtree Willey publications.
- 13. Inorganic Chemistry, J.E. Huheey, K.A.Keiter and R.L.Keiter 4 th Edition Harper Cottens College Publications (1993).
- 14. Homogeneous Catalysis by Metal complexes Vol I, M MTaqui Khan and A E Martell, Academic Press NY (1974).
- 15. Inorganic Chemistry, Keith F.Purcell and John C.Kotz, Holt-Saunders International Editions, London (1977).
- 16. Advanced Inorganic Chemistry 3rd, 5th & 6th Editions.: F.A. Cotton& G. Wilkinson:
- 17. Bioinorganic chemistry: Lippard S J Jeremy M Berg Stephen J Lippard, University Science Books ,Mill Valley, California, 1994.

Web resources:

Introduction to Organometallic Chemistry- <u>https://nptel.ac.in/courses/104101006</u> Advanced Transition Metal Organometallic Chemistry- <u>https://nptel.ac.in/courses/104101100</u> Advanced Transition Metal Chemistry- <u>https://onlinecourses.nptel.ac.in/noc22_cy60/course</u>

| M.Sc. (Chemistry) | First Year Semester- | I I [Level 6.0] |
|-------------------|----------------------|------------------|
|-------------------|----------------------|------------------|

| Code of the Course/ Subject | Title of the Course/Subject | (Total Number of Periods) |
|--------------------------------|---|------------------------------|
| CHE 203 | Basic Analytical Chemistry (DSC–II.2) | 45 hrs (3 hrs/week) |

Course Outcomes: At the end of the course, students will be able to:

- 1. demonstrate a comprehensive understanding of analytical chemistry principles and techniques
- 2. recognize and classify different analytical methods and sampling techniques, evaluating their applicability in various scenarios
- 3. analyze and interpret titration curves and thermograms, applying theoretical concepts to predict behaviour.
- 4. determine equilibrium constants and pH values accurately
- 5. comprehend polarography principles and use them to quantitate metal ions and organic compounds

Unit-I: Introduction and Sampling

- 1. Introduction to Analytical Chemistry
 - Types of analysis: qualitative and quantitative
 - Classification of analytical methods: classical and instrumental
- 2. Sampling and Sample Treatment
 - Criteria for obtaining a representative sample
 - Techniques for sampling gases, liquids, solids, and particulates
 - Sampling of hazardous materials and safety considerations
- 3. Sample Dissolution Methods for Elemental Analysis
 - Dry and wet ashing techniques
 - Acid digestion method
 - Fusion processes for sample dissolution
 - Dissolution methods for organic samples
- 4. Detection and Quantification
 - Concepts of sensitivity, limit of detection, and limit of quantification
 - Role of noise in determining the detection limit
 - Units used in chemical analysis and their interconversion

Unit-II: Volumetric Analysis (7 hours)

- 1. Volumetric Analysis: General Principles
 - Criteria for reactions used in titrations
 - Primary standards and secondary standards
 - Theory of indicators
- 2. Types of Titrations and Examples
 - Acid-base titrations
 - Precipitation titrations
 - Redox titrations
 - Complexometric titrations
- 3. Titration Curves and Indicators
 - Titration curves for monoprotic and polyprotic acids and bases
 - Indicators used in various types of titrations
 - Masking and demasking agents

Unit-III: Gravimetric Analysis (8 hours)

1. Gravimetric Analysis: General Principles

(7 hours)

- Conditions of precipitation and solubility product
- Precipitation equilibria
- 2. Steps Involved in Gravimetric Analysis
 - Gravimetric analysis of barium and nickel
 - Purity of precipitate: co-precipitation and post-precipitation
 - Fractional precipitation
- 3. Precipitation from Homogeneous Solution
 - Crystalline, gelatinous, and curdy precipitate
 - Peptization phenomena

Unit-IV: Conductometry (8 hours)

- 1. Conductometry: Concepts and Definitions
 - Electrical resistance, conductance, resistivity, and conductivity
 - Specific, molar, and equivalent conductance
 - Effect of dilution on conductance
- 2. Kohlrausch's Law and Applications
 - Kohlrausch's law and its significance
 - Applications in determination of dissociation constant, solubility product
- 3. Conductometric Titrations
 - Different types of conductometric titrations
 - High-frequency titrations
 - Numerical problems

Unit-V: Potentiometry (8 hours)

- 1. Potentiometry: Principles and Electrodes
 - Circuit diagram of a simple potentiometer
 - Indicator electrodes: hydrogen electrode, quinhydrone electrode, antimony electrode, glass electrode
 - Reference electrodes: calomel electrode, Ag/AgCl electrode
- 2. Theory of Potentiometric Titrations
 - Acid-base, redox, precipitation, and complexometric titrations
 - Nernst equation, standard electrode potential, determination of cell potential, n, Kf, Ksp
- 3. pH Titration and Buffer Solutions
 - Buffer solutions and buffer capacity
 - Calculation of pH of buffer mixtures using the Henderson-Hasselbalch equation

Unit-VI: Polarography (7 hours)

- 1. Polarography: Principles and Instrumentation
 - Principle of DC polarography
 - Instrumentation in polarography: DME, advantages, limitations
- 2. Types of Currents in Polarography
 - Residual, migration, diffusion, limiting, adsorption, kinetic, catalytic currents
 - Ilkovic equation: diffusion current constant and capillary characteristics
- 3. Polarographic Wave and Half Wave Potential
 - Derivation of the equation of the polarographic wave
 - Experimental determination of half-wave potential
- 4. Types of Electrode Reactions in Polarography
 - Reversible, quasi-reversible, and irreversible electrode reactions
 - Polarographic maxima and maximum suppressor
- 5. Applications of Polarography
 - Determination of dissolved oxygen

- Metal ion quantification and speciation •
- Simultaneous determination of metal ions •
- Analysis of organic compounds
- Limitations of polarography •

Course Material/Learning Resources:

Textbooks:

- "Analytical Chemistry: Problems and Solutions" by S. M. Khopkar (New Age International Publication) 1.
- 2. "Basic Concepts in Analytical Chemistry" by S. M. Khopkar (New Age International Publication)

Reference Books:

- 1. "Quantitative Analysis" by Day and Underwood (Prentice-Hall of India)
- 2. "Vogel's Textbook of Quantitative Inorganic Analysis" by Bassett, Denney, Jeffery, and Mendham (ELBS)
- 3. "Analytical Chemistry" by Gary D. Christian (Wiley, India)
- 4. "Instrumental Methods of Analysis" by Willard, Merrit, Dean, Settle (CBS Publishers, Delhi, 1986)
- 5. "Instrumental Methods of Chemical Analysis" by Braun (Tata McGraw-Hill)
- 6. "Advanced Analytical Chemistry" by Meites and Thomas (McGraw-Hill)
- 7. "Instrumental Methods of Analysis" by G. Chatwal and S. Anand (Himalaya Publishing House)
- 8. "Fundamentals of Analytical Chemistry" by S. A. Skoog and D. W. West (Saunders College Publishing)

Additional Online Resources:

1. OpenCourseWare - MIT: Access free lecture notes, assignments, and exams from the Massachusetts Institute of Technology's analytical chemistry courses.

Journals:

- 1. Analytical Chemistry (American Chemical Society)
- 2. Journal of Analytical Chemistry (Springer)
- 3. Talanta (Elsevier)
- 4. Analytica Chimica Acta (Elsevier)
- 5. Journal of Chromatography A/B (Elsevier)

| M.Sc. (Chemistry) | First Year Semester- | I I [Level 6.0] |
|-------------------|----------------------|------------------|
|-------------------|----------------------|------------------|

| Code of the Course/ Subject | Title of the Course/Subject | (Total Number of Periods) |
|--------------------------------|--|------------------------------|
| CHE 204 (i) | Photo-inorganic chemistry and Organometallics (DSE–II (i)) | 60 hrs (4 hrs/week) |

Course Outcomes: At the end of the course, students will be able to:

- 1. Explain photochemical laws, quantum yield, and the concept of electronically excited states and their lifetimes.
- 2. Describe the principles and applications of flash photolysis and stopped flow techniques for studying photochemical reactions.
- 3. Analyze the processes of energy dissipation by radiative and non-radiative pathways in excited states.
- 4. Analyze the electronically ligand field excited states of metal complexes containing d1 to d10 configurations.
- 5. Describe the structures and bonding of organotransition compounds with multicenter bonds, including alkenes, alkynes, allenes, and cyclic π -metal complexes.
- 6. Explain the reactions of transition metal-carbenes, -carbynes, and -bridging carbenes, including ligand substitution and nucleophilic and electrophilic attack.
- 7. Analyze the mechanism and importance of Wilkinson's catalyst in the hydrogenation of olefins.

Unit-I:

A) Basics of Photochemistry:

Basics of photochemical processes: Absorption, excitation, photochemical laws, quantum yield, Frank-Condon principles; Photochemical stages-primary & secondary processes, electronically excited states-life times-measurements of the times; Flash photolysis and stopped flow techniques; Energy dissipation by radiative and non-radiative processes

B) Properties of excited states:

Photochemical kinetics, Calculation of rates of radiative processes.

Unit II: Ligand field photo chemistry of transition metal complexes

Electronically ligand field excited states of metal complexes containing d¹ to d¹⁰ configuration, Photochemistry of Cr(III)complexes: Photo-substitutions reactions, Photo aquation reactions, photorecimization reactions, Adamson's rules for photoreactions; Photochemistry of Co(III) complexes: Introduction, energy level diagram, photoaquations and photoredox reactions in Co(III) amine, Co(III) cyanide complexes, photoisomerization; Photo redox properties of Ru(III), Ce(III) and Ce(IV) complexes; Application of redox processes of electronically excited states for catalytic purposes.

UNIT III : Photochemical reaction on solid surface

Introduction, basic principle of photocatalysis, photocatalysts, photoreactive oxides;

Relation between solar spectrum & band gap, acceptor and donor level of photocatalyst, generation of electron-holepair; Needs of modification of photocatalysts, semiconductor supported metal oxide systems, synthesis methods, Characterization, water photolysis;

Application of photocatalytic materials for degradation of organic pollutants, Nitrogen fixation & carbon dioxide reduction.

UNIT IV: Organotransition compounds

Structures of organotransition compounds with multicenter bonds (non-classically bonded): Concept of hapticity, transition metal complexes of alkenes, Ziese salt, allenes, alkynes, allyls, butadienes; cyclic π -metal complexes of cyclobutadienes, cyclopentadienyls, arenes,

10 hrs

10 hrs

10 hrs

49

10 hrs

cycloheptatrienyls and cyclooctatetraenes; structure and bonding in ferrocene; stereochemical non-rigidity in organometallic compounds and fluxional compounds, structures of bimetallic and cluster complexes.

Unit-V: Organotransition metal chemistry

 σ -Bonded transition metal-alkyls, -aryls, -alkenyls(vinyls), -alkynyls(acetylides), reactions in σ organyls - homolytic cleavage, Oxidative addition, Intramolecular Oxidative addition, Oxidative addition M-M multiple bond, Oxidative Coupling, reductive elimination, electrophilic cleavage, insertion, β -metal hydrogen elimination, α -abstraction or α -elimination; Transition metalcarbenes, -carbynes, -bridging carbenes and -carbynes, reactions of carbene/ and carbyne complexes ligand substitution, nucleophilic, electrophilic attack, dismutation and ligand coupling reactions.

UNIT-VI: Organometallics as catalysts

Importance of organometallic compounds as catalysts, Condition to be satisfied by metal to act as catalyst, importance of Willkinsons catalyst in hydrogenation of olefins, mechanism; hydroformylation of olefins-the oxo process by HCo(CO)₄, mechanism, modification and mechanism of modified catalyst over original catalyst; Oxidation of olefins by Wacker's process, mechanism; synthesis of chiralpharmaceuticals, Olefin metathesis, heterogeneous catalysis: Ziegler Natta polymerization, Water gas shif reaction, mechanism; coupling reactions - Suzuki coupling, Heck coupling and related cross coupling reactions.

Course Material/Learning Resources

- 1. Elschenbroich Ch.and Salzer A.: Organometallics, VCH, Weinheim, NY.
- 2. Balzani Vand Cavassiti V.: Photochemistry of Coordination compounds, AP, London
- 3. Purcell K.F.and KotzJ.C., An Introduction to Inorganic Chemistry, Holt Sounder, Japan.
- 4. Rohtagi K.K.and Mukharjee, Fundamentals of Photochemistry, Wiley eastern
- 5. Calverts J.G.and Pits.J.N., Photochemicals of Photochemistry, John Wiley
- 6. Wells, Introduction of Photochemistry
- 7. Paulson, Organometallic Chemistry, Arnold
- 8. Rochow, Organometallic Chemistry, Reinhold
- 9. Zeiss, Organometallic Chemistry, Reinhold
- 10. Gilbert A.and Baggott, J, Essential of Molecular Photochemistry, Blackwell Sci. Pub.
- 11. Turro N.J.and Benjamin W.A., Molecular Photochemistry
- 12. CoxAand Camp, T.P. Introductory Photochemistry, McGraw-Hill
- 13. KundallR.P.and GilbertA,Photochemistry, Thomson Nelson Coxon J and Halton
- 14. Organic Photochemistry, Cambridge University Press.

10 hrs

10 hrs

| Code of the Course/ Subject | Title of the Course/Subject | (Total Number of Periods) |
|--------------------------------|-----------------------------|------------------------------|
| CHE 204 (ii) | Advanced Organic Chemistry | 60 hrs |
| | (DSE–II (ii)) | (4 hrs/week) |

Course Outcomes: At the end of the course, students will be able to:

- 1. Analyse the mechanisms and synthetic applications of various molecular rearrangements
- 2. Discuss the formation of C-C and C-X single bonds through name reactions.
- 3. Design the construction of double and multiple bonds through various name reactions,
- 4. Explain the carbonyl methylenation using reagents such as Tebbe reagent, Petasis reagent, and Nystedt reagent.
- 5. Analyse the preparation and synthetic applications of enamines, focusing on the Stork enamine reaction.
- 6. Utilize the synthetic application of organometallic reagents for achieving molecular complexity

Unit I Molecular rearrangement:

Electron deficient carbon: Pinacol-Pinacolone, Semi-Pinacol Wagner- Meerwein, Tiffenev –Demjnov ring expansion, and Arndt-Eistert synthesis, Dienone-phenol rearrangement, Wolf rearrangement.

Electron deficient nitrogen: Hofmann, Lossen, Curtius, Schmidt, Neber, Stieglitz and Beckmann rearrangements.

Base catalysed rearrangements: Benzil-Benzilic acid, Favorskii, Sommlett-Hauser and Pummerer rearrangement,

Fragmentation reactions: Electron push and pull requirement, Beckmann, Eschenmoser, Alicyclic-Grobb fragmentation.

Unit II Organic name Reaction:

(10 Hrs)

Formation of Double and multiple bond reaction: Julia–Lythgoe olefination, Julia-Kocienski Olefination, Peterson olefination, Shapiro reaction, Bamford-Stevens reaction, Corey–Winter olefination, Ramberg–Bäcklund reaction, Takai olefination. Corey-Fuchs Reaction

Formation of C-C and C-X single bond reaction: Cannizzaro reaction, Mannich reaction, Mukaiyama aldol reaction, Reformatsky reaction, Ritter reaction, Stetter Reaction, Appel reaction, Mitsunobu reaction, Houben–Hoesch reaction.

Unit III Ylides and Enamines:

(10 Hrs)

Phosphorus and Sulphur ylides: Preparation, synthetic applications with stereochemistry, Wittig reaction, Schlosser wittig reaction, Horner-Wadsworth-Emmons Reaction, Corey–Chaykovsky reaction.

Enamine: Preparation, synthetic applications with stereochemistry,Stork enamine reaction. **Carbonyl methylenation**: Tebbe reagent, Petasis reagent, Nystedt reagent.

Unit IV Formation of carbon-carbon bonds via organometallic reagents (10 Hrs) Preparation and synthetic applications of organolithium reagents, organomagnesium reagents, organocopper reagents, organochromium reagents, organozinc reagents, organotitanium reagents, and organoborane reagents.

Unit V C-C, C-X coupling reactions and metallocene: (10 Hrs)

(10L)

Suzuki coupling, Heck coupling, Stille coupling, Sonogashira cross-coupling, Buchwald-Hartwig coupling, Negishi-Kumada coupling, Trost T-suji coupling, Kumada Coupling, Hiyama coupling.

Metallocene: Applications of metallocene based on Fe and Cr.

Unit VI Grubb's Metathesis and Transition metal complexes in organic synthesis: (10 Hrs) Grubb's Metathesis:

Preparation and synthetic applications of metathesis reaction of alkene and alkyne. RCM (ring closing metathesis), ROM (ring opening metathesis), Cross metathesis, Ene-yne metathesis.

Transition metal complexes in organic synthesis:

Reppe reaction, Pauson–Khand reaction, Nicholas reaction, Hydroformylation (Oxo process) and Waker Process, Collman's Reagent

Course Material/Learning Resources:

- 1. Organic Chemistry" by Jonathan Clayden, Nick Greeves, and Stuart Warren
- 2. "Advanced Organic Chemistry" by Francis A. Carey and Richard J. Sundberg
- 3. "Organic Chemistry" by Paula Yurkanis Bruice
- 4. "Modern Organic Synthesis: An Introduction" by Michael H. Nantz and G. Marc Loudon
- 5. "Protecting Groups" by Philip J. Kocienski:
- 6. "Phosphorus Ylides: Chemistry and Applications in Organic Synthesis" edited by Oleg I. Kolodiazhnyi
- 7. "Sulfur Ylides: Emerging Synthetic Intermediates" edited by Michael P. Doyle and Richard A. Batey.
- 8. "Organic Synthesis: Strategy and Control" by Paul Wyatt and Stuart Warren
- 9. "Oxidation in Organic Chemistry" by K. Barry Sharpless and Michael G. Finn
- 10. "Reduction of Organic Compounds: Theory and Practice" by A. Zaks and A. B. Sowers
- 11. "Name Reactions and Reagents in Organic Synthesis" by Bradford P. Mundy, Michael G. Ellerd, and Frank G. Favaloro Jr.
- 12. "Strategic Applications of Named Reactions in Organic Synthesis" by Laszlo Kurti and Barbara Czako.
- 13. "Comprehensive Organic Name Reactions and Reagents" edited by Zerong Wang
- 14. "The Art of Writing Reasonable Organic Reaction Mechanisms" by Robert B. Grossman.
- 15. "Principle of Organic Synthesis" by R. O. C Norman and J. H. Coxon, 1st Ed, ELBS, 1993.
- 16. "Organic synthesis" by Micheal B Smith
- 17. "Modern methods of organic synthesis" by W. Carruthers
- 18. "Principle of Organic Synthesis" by R. O. C Norman and J. H. Coxon, 1st Ed, ELBS, 1993.
- 19. "Reagents for Organic synthesis" by L. W. Paqueette (Ed), John Wiley, 1995.
- 20. "Handbook of Reagents for Organic Synthesis: Reagents for Heteroarene Synthesis" by Andre B. Charette, Wiley-Blackwell, 1 edition, 2017.
- 21. "Protective Groups in Organic Synthesis" by T.W. Greene Wiley-VCH, 1999. 2. B. P.
- 22. "Name Reactions and Reagents in Organic Synthesis" by Mundy, M. G. Ellerd, and F. G. Favaloro Jr., Wiley, 2nd Ed. 1988.

Web Resources

1. Organic Syntheses: Organic Syntheses is a peer-reviewed journal that publishes detailed experimental procedures for various organic transformations, including Name Reactions. You can access their website here: <u>https://www.orgsyn.org/</u>

- 2. Organic Chemistry Portal Name Reactions: The Organic Chemistry Portal offers a comprehensive collection of articles, reviews, and resources on various Name Reactions in organic synthesis. You can access it here: https://www.organic-chemistry.org/namedreactions/
- 3. Organic Chemistry Portal Reagents in Organic Synthesis: The Organic Chemistry Portal also provides a section on Reagents in Organic Synthesis, where you can find information on various reagents used in organic transformations. You can access it here: <u>https://www.organic-chemistry.org/topics/reagents/</u>
- 4. <u>Reagents in Organic Synthesis https://onlinecourses.nptel.ac.in/noc21_cy42/preview</u>
- 5. Principles of Organic Synthesis <u>https://onlinecourses.nptel.ac.in/noc21_cy41/preview</u>

| Code of the Course/ Subject | Title of the Course/Subject | (Total Number of Periods) |
|--------------------------------|--|------------------------------|
| CHE 204 (iii) | Electrochemical Processes and Applications (DSE–II (iii)) | 60 hrs (4 hrs/week) |

M.Sc. (Chemistry) First Year Semester- II [Level 6.0]

Course Outcomes: At the end of the course, students will be able to:

- 1. Define and explain the key terms and concepts in electrochemistry.
- 2. Balance redox equations and determine the standard electrode potentials.
- 3. Calculate cell EMF and understand the thermodynamic feasibility of electrochemical reactions.
- 4. Apply the Nernst equation to analyze the effects of temperature and concentration on cell potential.
- 5. Describe the kinetics of electrode reactions using the Butler-Volmer equation and the Tafel plot.
- 6. Analyze the factors influencing the reversibility of electrochemical processes.
- 7. Understand the principles and applications of electrochemical instrumentation and techniques.
- 8. Explain the structure and dynamics of electrical double layers and their role in energy devices.
- 9. Differentiate between Faradaic and non-Faradaic charging mechanisms in energy storage systems.
- 10. Discuss the working principles and mechanisms of operation of electrochemical capacitors.
- 11. Evaluate the materials development and advancements in supercapacitor technology.
- 12. Describe the redox reactions and operation mechanisms of batteries, including metal-ion and metal-based rechargeable batteries.
- 13. Discuss the evolution of battery technologies and emerging trends.
- 14. Understand the principles and challenges of battery management systems.
- 15. Identify real-life applications of electrochemical processes in energy storage, renewable energy systems, and electronic devices.

UNIT I: Basics of Electrochemical Processes and Thermodynamics of Cells 10 h

Basics of Electrochemical Processes

- 1. General electrochemical concepts
 - Definition and scope of electrochemistry
 - Importance of electrochemical processes in various fields
 - Key terms and definitions in electrochemistry
- 2. Redox reactions
 - Oxidation and reduction processes
 - Balancing redox equations
 - Redox couples and their notation
- *3. Reference electrodes*

- Purpose and function of reference electrodes
- Standard hydrogen electrode (SHE) and other reference electrodes
- Construction and potential measurement of reference electrodes
- 4. Galvanic and electrolytic cells
 - Distinction between galvanic and electrolytic cells
 - Cell notation and representation of cell reactions
 - Cell potential and EMF (Electromotive Force)

Thermodynamics of Electrochemical Cells

- 1. Electrode potentials
 - Standard electrode potentials and their determination
 - Significance of electrode potentials in redox reactions
- 2. Half reactions and reduction potentials
 - Definition and representation of half reactions
 - Reduction potentials and their relation to standard electrode potentials
- 3. Reversibility
 - Reversible and irreversible electrochemical processes
 - Factors influencing the reversibility of reactions
- 4. Free energy and cell EMF
 - Relationship between free energy and cell EMF
 - Calculation of ΔG and ΔG° from cell potential
- 5. Nernst Equation
 - Derivation and applications of the Nernst equation
 - Temperature and concentration dependence of cell potential
- 6. Liquid junction potentials
 - Causes and effects of liquid junction potentials
 - Mitigation strategies for liquid junction potential effects

UNIT II: Kinetics of Electrode Reactions

- 1. Homogeneous kinetics
 - Rate equations and rate constants for homogeneous reactions
 - The Arrhenius equation and its significance in electrochemistry
- 2. Butler-Volmer model of electrode kinetics
 - Derivation and interpretation of the Butler-Volmer equation
 - Influence of overpotential on electrode kinetics
- 3. The standard rate constant and the transfer coefficient
 - Definition and determination of the standard rate constant
 - Relationship between the transfer coefficient and electrode kinetics
- 4. Microscopic theories of charge transfer
 - Introduction to Marcus theory and its application to electron transfer reactions
 - Concepts of electron tunneling and reorganization energy
- 5. Tafel plot
 - Interpretation and application of Tafel plots in electrochemical kinetics
 - Determination of rate constants and reaction mechanisms
- 6. Multistep electrode reactions
 - Description and analysis of multistep electrode reactions
 - Rate-determining steps and reaction intermediates
- 7. Charge transfer at electrode-solution interfaces
 - Description of charge transfer processes at the electrode-electrolyte interface

10h

10h

- Influence of adsorption and surface phenomena on electrode reactions
- 8. Quantization of charge transfer
 - Introduction to charge quantization and its implications in electrochemical reactions

UNIT III: Mass Transfer and Electrical Double Layers

Mass Transfer by Migration and Diffusion

- 1. General mass transfer equation
 - Overview of mass transfer phenomena in electrochemical systems
 - Governing equations for migration and diffusion processes
- 2. Migration
 - Definition and mechanisms of migration in electrolytes
 - Migration velocities and their dependence on electric field and ion mobility
- 3. Diffusion
 - Fick's Laws of diffusion and their applications in electrochemistry
 - Diffusion coefficients and concentration profiles in solutions
- 4. Combined migration and diffusion
 - Effects of migration and diffusion on species distribution near electrodes
 - Concentration polarization and its consequences in electrochemical cells

Electrical Double Layers

- 5. Electrical Double Layers
 - Introduction to electrical double layers (EDL)
 - Components of EDL: Stern layer and diffuse layer
 - Charge distribution and potential distribution across the EDL
- 6. Structure and Dynamics of Double Layers
 - The Gouy-Chapman theory and the concept of surface potential
 - The Helmholtz layer and the development of the Stern layer
 - Effect of electrolyte concentration on the EDL structure
- 7. Faradaic and Non-Faradaic Charging Mechanisms
 - Faradaic processes: Redox reactions at the electrode-electrolyte interface
 - Non-Faradaic processes: Ion adsorption/desorption without redox reactions
 - Contribution of Faradaic and non-Faradaic processes to charge storage

UNIT IV: Electrochemical Instrumentation and Techniques

- 1. Linear sweep voltammetry
 - Principles and applications of linear sweep voltammetry
 - Determination of electrochemical parameters from voltammograms
- 2. Cyclic voltammetry
 - Basics of cyclic voltammetry and its experimental setup
 - Interpretation of cyclic voltammograms and identification of redox processes
- 3. Chronopotentiometry
 - Principles and applications of chronopotentiometry
 - Measurement of current and potential transients
- 4. Chronoamperometry
 - Theory and applications of chronoamperometry
 - Analysis of current-time transients and determination of rate constants
- 5. Concepts of impedance
 - Introduction to impedance spectroscopy and its principles
 - Interpretation of impedance spectra and determination of electrochemical parameters

UNIT V: Electrochemical Capacitors

10h

- 1. Generation and Storing of Charges
 - Introduction to electrochemical capacitors (ECs)
 - Mechanisms of charge storage in ECs
 - Double-layer capacitance and pseudocapacitance
- 2. Derivation of Capacitance Equations
 - Derivation of the parallel-plate capacitor equation
 - Extended capacitance equations for ECs
 - Relationship between charge, voltage, and capacitance
- 3. Evolution of Capacitor Technologies
 - Historical development of capacitor technologies
 - Advancements in ECs and their applications
- 4. Materials Development for Supercapacitors
 - Electrode materials for ECs
 - Carbon-based materials (activated carbon, carbon nanotubes)
 - Transition metal oxides and conducting polymers
 - Hybrid and composite electrode materials
- 5. Working Principles and Mechanism of Operation
 - Electrode-electrolyte interface and electrical double layer (EDL)
 - Faradaic and non-Faradaic charge storage mechanisms
 - Ion adsorption and ion desorption processes
- 6. Real-life Applications of Supercapacitors
 - Energy storage in renewable energy systems
 - Power backup and peak load management
 - Electric vehicle applications
 - Hybrid energy storage systems
 - Portable electronic devices
 - Industrial and grid-scale applications

UNIT VI: Batteries

- 1. Redox Reactions in Batteries
 - Introduction to redox reactions in electrochemical cells
 - Oxidation and reduction half-reactions in batteries
 - Electrode materials and their redox properties
- 2. Cell EMF
 - Definition and significance of cell electromotive force (EMF)
 - Calculation of cell EMF using standard reduction potentials
 - Relationship between cell EMF and thermodynamic feasibility
- 3. Evolution of Battery Technologies
 - Historical development of battery technologies
 - Primary and secondary batteries
 - Advancements and emerging trends in battery technology
- 4. Operation Mechanism of a Battery
 - Basic components of a battery: electrodes, electrolyte, and separator
 - Working principles of galvanic cells and rechargeable batteries
 - Charge and discharge processes in a battery
- 5. Advanced Batteries Metal-Ion and Metal-Based Rechargeable Batteries
 - Overview of metal-ion batteries (e.g., lithium-ion batteries)
 - Electrode materials and redox reactions in metal-ion batteries

10h

- Challenges and advancements in metal-ion battery technology
- Introduction to metal-based rechargeable batteries (e.g., sodium-ion, magnesium-ion batteries)
- Electrode materials and redox reactions in metal-based batteries
- 6. Battery Management Systems
 - Overview of battery management systems (BMS)
 - Battery charging and discharging control strategies
 - State-of-charge (SOC) and state-of-health (SOH) estimation
 - Battery safety and protection mechanisms

Text & Reference Books & Journals:

- 1. Bard, A. J., & Faulkner, L. R. (2000). Electrochemical Methods: Fundamentals and Applications (2nd ed.). Wiley.
- 2. Newman, J., & Thomas-Alyea, K. (2012). Electrochemical Systems (3rd ed.). Wiley.
- 3. Compton, R. G., Banks, C. E., & Meadows, R. (2018). Understanding Voltammetry: Simulation of Electrode Processes (4th ed.). World Scientific Publishing.
- 4. Wang, J. (2008). Electrochemical Supercapacitors: Scientific Fundamentals and Technological Applications. Springer.
- 5. Argyropoulos, P., Gude, V. G., & Katsaounis, A. (Eds.). (2019). Redox Flow Batteries: Fundamentals and Applications. Elsevier.
- 6. Armand, M., & Tarascon, J. M. (2008). Building better batteries. Nature, 451(7179), 652-657.
- 7. Bruce, P. G., Freunberger, S. A., & Hardwick, L. J. (2012). Li-O2 and Li-S batteries with high energy storage. Nature Materials, 11(1), 19-29.
- 8. Goodenough, J. B., & Park, K. S. (2013). The Li-ion rechargeable battery: A perspective. Journal of the American Chemical Society, 135(4), 1167-1176.
- 9. Tarascon, J. M., & Armand, M. (2001). Issues and challenges facing rechargeable lithium batteries. Nature, 414(6861), 359-367.

| Code of the Course/ Subject | Title of the Course/Subject | (Total Number of Periods) |
|--------------------------------|---|------------------------------|
| CHE 204 (iv) | Thermal and Electro-Analytical Techniques (DSE–II (iv)) | 60 hrs (4 hrs/week) |

M.Sc. (Chemistry) First Year Semester- II [Level 6.0]

Course Outcomes: At the end of the course, students will be able to:

- 1. Define and explain the key terms and concepts in advanced analytical techniques, including thermogravimetry, voltammetry, ion-selective electrodes, and coulometry.
- 2. demonstrate proficiency in operating sophisticated instruments, interpreting complex data, and performing thermogravimetric titrations
- 3. analyze electrochemical data and apply it for quantitative analysis of metals and anions
- 4. develop skills in minimizing polarization effects in electrogravimetric measurements and utilizing electrochemical microscopy for nanoscale analysis
- 5. gain the expertise to solve intricate analytical problems across diverse fields

Unit-I: Thermogravimetry (10h)

Introduction to Different Thermal Methods:

• Overview of various thermal analysis techniques

- Thermogravimetry (TG and DTG)
- Static thermogravimetry
- Quasistatic thermogravimetry
- Dynamic thermogravimetry

Instrumentation:

- Balances for accurate measurements
- X-Y recorder for data visualization
- Stanton-Redcroft TG-750 instrument for thermogravimetry analysis
- Thermogram and its interpretation
- Factors influencing thermogram patterns

Applications of Thermogravimetry:

• Practical applications of thermogravimetry in different fields

Thermogravimetric Titration:

- Theoretical foundations of thermogravimetric titration
- Instrumentation involved in thermogravimetric titration
- Applications of thermogravimetric titration in analytical chemistry

Unit-II: Differential Thermal Analysis and Differential Scanning Calorimetry (10h)

Differential Thermal Analysis (DTA):

- Theories underlying differential thermal analysis
- DTA curves and their interpretation
- Factors affecting DTA curves
- Applications of DTA in thermal analysis
- Simultaneous determination in thermal analysis

Differential Scanning Calorimetry (DSC):

- Introduction to differential scanning calorimetry
- Instrumentation used in DSC analysis
- DSC curves and their interpretation
- Factors influencing DSC curves
- Applications of DSC in various industries

Unit-III: Voltammetry and Electrochemical Analysis (10h)

- 1. Stripping Voltammetry: Principles and techniques in anodic and cathodic stripping voltammetry
- 2. Applications of stripping voltammetry in metal ion analysis
- 3. Limitations of stripping voltammetry
- 4. Adsorptive stripping voltammetry: Principles, techniques, and applications in metal ion and organic analysis
- 5. Advantages of adsorptive stripping voltammetry over anodic stripping voltammetry
- 6. Catalytic effects in voltammetry
- 7. Working electrodes: Mercury electrodes, carbon electrodes, film electrodes
- 8. Cyclic voltammetry: Principles, techniques, Randles-Sevcik equation, interpretation of voltammogram (reversible, irreversible, and quasi-reversible systems)
- 9. Applications of cyclic voltammetry in the study of reaction mechanisms and adsorption processes
- 10. Comparison of voltammetry with AAS and ICP-AES

Unit-IV: Ion Selective Electrodes (10h)

- 11. Ion selective electrodes: Theory of membrane potential, types of ion-selective electrodes
- 12. Construction of solid-state electrodes, liquid membrane electrodes, glass membrane electrodes, and enzyme electrodes
- 13. Selectivity coefficients
- 14. Glass electrodes with reference to $\mathrm{H}^{\scriptscriptstyle +},\,\mathrm{Na}^{\scriptscriptstyle +},\,\mathrm{and}\;\mathrm{K}^{\scriptscriptstyle +}$ ions
- 15. Applications of ion selective electrodes in the analysis of environmentally important anions (F⁻, Cl⁻, Br⁻, I⁻, NO₃⁻, CN⁻)
- 16. Advantages of ion selective electrodes

Unit-V: Electrogravimetry (10h)

• *Electrogravimetric Analysis:* Introduction to electrogravimetry and its principles, Electrodeposition mechanisms in electrogravimetry

- *Polarization and Electrogravimetry:* Polarization effects in electrogravimetric measurements, Minimizing polarization in electrogravimetry
- *Types of Electrogravimetric Methods:* Constant current electrolysis in electrogravimetry, Constant potential electrolysis in electrogravimetry
- *Application of Electrogravimetry:* Examples of electrogravimetry applications in analysis, Environmental, metallurgical, and quality control applications

Unit-VI:Coulometry and Electrochemical Microscopy (10h)

- *Coulometry: Principles and Techniques:* Introduction to coulometry and its principles, Faraday's laws and their application in coulometry
- *Types of Coulometric Methods:* Controlled potential coulometry (potential coulometry), Constant current coulometry (amperostatic coulometry)
- *Application of Coulometry:* Overview of coulometric titrations and their applications, Analysis of pharmaceuticals, metals, and other substances using coulometry
- Introduction to electrochemical microscopy: Scanning probe microscopy (SPM), scanning tunneling microscopy (STM), atomic force microscopy (AFM), scanning electrochemical microscopy (SECM)

Textbook & Reference Books:

- 1. Skoog, D. A., Holler, F. J., & Crouch, S. R. (2017). Principles of Instrumental Analysis. Cengage Learning.
- 2. Brown, M. E., & Gallagher, P. K. (2016). Introduction to Thermal Analysis: Techniques and Applications. Springer.
- 3. Bard, A. J., & Faulkner, L. R. (2000). Electrochemical Methods: Fundamentals and Applications. Wiley.
- Kissinger, P. T., & Heineman, W. R. (1996). Laboratory Techniques in Electroanalytical Chemistry. CRC Press.
- 5. IUPAC. (2009). Compendium of Analytical Nomenclature: Definitive Rules 2007 (3rd ed.). The Royal Society of Chemistry.
- 6. Fritz, J. S., & Schenk, G. H. (2003). Handbook of Electrochemistry. Wiley-VCH.
- 7. Šesták, J., & Berggren, G. (2014). Thermal Analysis of Polymeric Materials. CRC Press.

| Code of the Course/ Subject | Title of the Course/Subject | (Total Number of Periods) |
|--------------------------------|------------------------------------|------------------------------|
| CHE 204 (v) | Unit Processes and Green Chemistry | 60 hrs |
| | (DSE–II (ii)) | (4 hrs/week) |

M.Sc. (Chemistry) First Year Semester- II [Level 6.0]

Course Outcomes: At the end of the course, students will be able to:

- 1. Analyze the mechanisms and synthetic applications of various molecular The mode of action of various agents used during organic process synthesis.
- 2. Apply the knowledge to established mechanism of unit processes.
- 3. The operational mechanism of various industrial equipment used in unit processes.
- 4. The basic principles of green chemistry.
- 5. To apply the knowledge to synthesis material by green method.

Unit I:

10 Hrs.

A) Nitration: Introduction, nitrating agents, batch and continuous nitration, kinetics and mechanism of aromatic nitration manufacturing and mechanism of nitrobenzene, Ortho and para nitro-chlorobenzene, para nitro acetanilide.

B) Alkylation: Introduction, types of alkylation, alkylating agents, factors affecting alkylation, manufacturing and mechanism of ethyl benzene, phenyl ethyl alcohol

Unit II:

A) Halogenation: introduction, halogenating agents, kinetics and thermodynamics of halogenation reaction, aromatic halogenation, photo-halogenation, manufacturing and mechanism of chlorobenzene, di-chloro fluro methane, mono-chloro acetic acid.

B) Amination by reduction: Introduction, methods of reduction, metal & acid, sulphide reduction, metal & alkali reduction, manufacturing and mechanism of aniline, meta nitro aniline, para amino phenol.

Unit III:

A) Sulphonation: Introduction, sulphonating agents, factors affecting sulphonation, industrial equipment used for sulphonation, desulphonation reaction, manufacturing and mechanism of benzene sulphonic acid, sulphonation of anthraquinone.

B) Oxidation: Introduction, oxidizing agents, vapour & liquid phase oxidation, kinetics and thermodynamics of oxidation reaction, manufacturing and mechanism of acetic acid, acetaldehyde, benzoic acid.

Unit IV:

A) Esterification: Introduction, esterification of organic acid, esterification of carboxylic acid derivatives, esters of inorganic acids, manufacturing and mechanism of ethyl acetate, vinyl acetate.

B) Hydrogenation: Introduction, catalysts used for hydrogenation, catalytic hydrogenation, kinetics and thermodynamics of hydrogenation reaction, manufacturing and mechanism of methanol from carbon monoxide and hydrogen, mechanism of hydrogenation of vegetable oil.

Unit V:

A) Hydrolysis: Introduction, mechanism and thermodynamics of hydrolysis, hydrolyzing agents, mechanism of hydrolysis of ethyl acetate, manufacturing of phenol from regenerative process.

B) Amination by Ammonolysis: Introduction, aminating agents, physical and chemical factors affecting ammonolysis, catalyst used in amination reaction, kinetics and thermodynamics of ammonolysis, manufacturing and mechanism of aniline from chlorobenzene, manufacturing of methyl amine from methanol.

Unit VI:

Green Chemistry and Green Synthesis: Introduction, Principles and Concepts of Green Chemistry.

A) Atom economic reactions - Rearrangement reactions, Addition reactions.

B) Atom un-economic reactions - Substitutions reactions, Elimination reactions, Witting reaction C) Reducing toxicity - Measuring toxicity.

Synthesis involving basic principle of Green Chemistry - Introduction, Synthesis of Styrene, Adipic acid, Urethane, Aromatic amine, Selective alkylation of active methylene group, Synthesis of Acetaldehvde, Furfural from biomass, Synthesis of s-metalochlore (herbicide), Ibuprofane, Paracetamol.

10 Hrs.

10 Hrs.

10 Hrs.

10 Hrs.

10 Hrs.

Books Suggested:

- 1) Unit Process in Organic Synthesis, by P. H. Grogins.
- 2) Shreve s Chemical Process Industries edited by Austin, McGraw-Hill.
- 3) Dryden s outlines of Chemical Technology, edited by M.Gopal Rao and M.Sittig,
- 4) Industrial Chemistry by B.K.Sharma
- 5) Hand book of industrial chemistry Vol I & II K. H. Davis & F.S. Berner Edited by S.C. Bhatia, CBSpublishers.
- 6) Green Chemistry: Environmentally Benign Reactions" by V K Ahluwalia
- 7) New Trends in Green Chemistry" by V K Ahluwalia and M Kidwai.
- 8) Green Chemistry: An Introductory Text" by Mike Lancaster.

| Code of the Course/ Subject | Title of the Course/Subject | (Total Number of Periods) |
|--------------------------------|--------------------------------|------------------------------|
| CHE 205 | Inorganic Chemistry Laboratory | 60 hrs |
| | (Lab 03) | (4 hrs/week) |
| | (based on DSC–II.2) | |

M.Sc. (Chemistry) First Year Semester- II [Level 6.0]

Course Outcomes: At the end of the course students will be able to

- 1. Design the methodologies to develop ecofriendly and green technology for industry and research.
- 2. Develop methods and remedies for reactions with environmental pollution.
- 3. Improve scientific practical information orally and in writing.
- 4. Get awareness about laboratory safety and handling of chemicals.
- 5. Separate mixture into its constituent using physical and chemical methods of separation.

Part-A

Part-A

Preparation of inorganic compounds. It is expected that preparation should be carried out using tenets of GreenChemistry. Any one of the prepared compound may be characterized by elemental analysis/estimation or MWdetermination or decomposition temperatures or molar conductance studies. (Any Five)

- 1. Preparation of [VO (acac)₂]
- 2. Preparation of bis(acetylacetonato)copper(II).
- 3. Preparation of tris (acetylacetonato) iron (III).
- 4. Preparation of tris (acetylacetonato) manganese (III).
- 5. Preparation of Isomers of Tris (8-Hydroxyquinolinato) aluminium (III)
- 6. Preparation of Potassium trioxalatomanganate(III), K₃[Mn(C₂O₄)₃]
- 7. Preparation of Cis and trans isomers of [Co(en)₂Cl₂]Cl

8. Preparation of Cis/Trans K [Cr(C₂O₄) 2(H₂O)₂].2H₂O potassium bisoxalatodiaquo chromate(III) dehydrate

- 9. Preparation of K_3 [Fe(C₂O₄)₃].3H₂O
- 10. Preparation of $[Co(Py)_2Cl_2]$
- 11. Preparation of [Ni(DMG)₂]
- 12. Preparation of [Cu₂(CH₃COO)₄(H₂O)₂]
- 13. Preparation of K $_3$ [Al (C₂O₄)₃](H₂O)₃

Part-B

Quantitative Analysis (Any two)

Quantitative analysis of mixture of cations involving their chemical separation and separate analysis of one cation by gravimetry and another by volumetric or colorimetric. Quantitative analysis of (Brass, Bronze and Dolamite)

Part-C Qualitative analysis (Eight mixtures)

Qualitative analysis of mixtures containing at least five radicals including interfering radicals (not more than one such

radical in a mixture), rare earth (not more than two rare earths in a mixture)

1. Cations of : Ag, Pb, Hg, Cu, Cd, Sn, Bi, As, Sb, Fe, Al, Cr, Co, Ni, Mn, Zn, Ca, Sr, Ba, Mg, Na, K and ammonium ion

2. Cations of rare elements: W, Tl, Mo, Ce, Ti, Th, Zr, U, V, Be and Li.

3. Interfering radicals: Phosphate, Oxalate, Fluoride and Tartrate.

Examination: CHE 205 Inorganic Chemistry Laboratory (Lab 03)

Time : 6-8 Hrs. (One day Examination)

Total Marks: 100

| А. | Exercise-I (Preparation) | 20 |
|----|--|-----------|
| В. | Exercise-II (Quantitative or Qualitative Analysis) | 20 |
| C. | Viva (External + Internal) | 10 |
| Е. | Internal assessment* | 50 |
| | Total | 100 |

*- Internal assessment will be continuous and based on the performance of a student throughout the session along with satisfactory submission of the term work

Course Material/Learning Resources:

- 1. Experiments and technique in organic experiments- D. Pasto, C. Johnson and M. Miller prentice Hall.
- 2. Macro- scale and micro-scale organic experiments-K.L. Williaman, D. C. Heath.
- 3. Systematic quantitative organic analysis H. Middleton, Edward Arnold.
- 4. Vogel's Textbook of practical organic chemistry Fifth Edition-Brain S. Furniss, Antoy J. Hannaford, Peter W,G. Smith, Austin R. Tatchell.
- 5. Qualitative organic Chemial analysis-A.I. Vogel.
- 6. Experiment organic chemistry Vol.I&II P.R. Singh, D. S. Gupta and K.S. Bajpai.
- 7. The Golden book of chemistry experiments- Robert Brent

Web resources:

- 1. Detection of functional group: <u>https://vlab.amrita.edu/index.php?sub=2&brch=191&sim=345&cnt=1</u>
- 2. Detection of element: https://vlab.amrita.edu/index.php?sub=2&brch=191&sim=344&cnt=1
- 3. Procedure for synthesis : <u>http://orgsyn.org/Default.aspx</u>

| Code of the Course/ Subject | Title of the Course/Subject | (Total Number of Periods) |
|--------------------------------|---------------------------------|------------------------------|
| CHE 206 | Analytical Chemistry Laboratory | 60 hrs |
| | (Lab 04) | (4 hrs/week) |
| | (based on DSC–III.2) | |

M.Sc. (Chemistry) First Year Semester- II [Level 6.0]

Course Outcomes: Upon completing this Analytical Chemistry Practical course, students will:

- 1. Demonstrate proficiency in classical methods and separation techniques, including calibration and statistical analysis.
- 2. Perform volumetric analysis to determine the concentration of various substances in mixtures and solutions.
- 3. Conduct gravimetric analysis to estimate the amount of specific substances in samples.
- 4. Master separation techniques like paper chromatography and ion exchange to separate metal ions.
- 5. Utilize electroanalytical techniques such as conductometric and potentiometric titrations for quantitative analysis.
- 6. Apply colorimetry to determine the dissociation constants of indicators and study complex formation.
- 7. Use instrumental methods to analyze commercial samples, such as vinegar, using conductometric titration.
- 8. Gain hands-on experience in various optical methods to estimate the concentrations of substances in solutions.
- 9. Develop essential skills in data interpretation, record keeping, and report writing for practical experiments

Section (A):

I. Calibration, validation, and computers

- (1) Calibration of pipette and burette.
- (2) Statistical analysis of data.
- (3) Use of MS-Excel in statistical analysis of data and curve fitting.

II. Volumetry

- (1) Determination of Na₂CO₃ in washing soda.
- (2) Estimation of nickel in given solution by direct complexometric titration with EDTA using bromopyrogallol red.
- (3) Estimation of nickel in given solution by complexometric back-titration with EDTA.
- (4) Estimation of chloride in given solution by Mohr's titration.
- (5) Estimation of chloride in given solution by Volhard's titration.
- (6) Determination of volume strength of commercial hydrogen peroxide by redox titration with KMnO4.
- (7) Estimation of Mn in the presence of Fe using masking phenomenon (ferromanganese alloy).

III. Gravimetry

- (1) Estimation of barium as barium sulphate.
- (2) Estimation of calcium as calcium oxalate/ calcium carbonate/ calcium oxide.

Section (B): Instrumental techniques

IV. Electroanalytical techniques

- (1) Analysis of commercial vinegar by conductometric titration.
- (2) Determination of strength of HCl and oxalic acid in a mixture conductometrically.
- (3) Determination of strength of oxalic acid and CH₃COOH in a mixture conductometrically.
- (4) Determination of degree of dissociation and dissociation constant of acetic acid conductometrically.
- (5) Estimation of phenol in dilute solution by conductometric titration with NaOH.
- (6) Determination of strength of HCl and CH₃COOH individually and in a mixture potentiometrically.

- (7) Determination of Fe(II) by potentiometric titration with $K_2Cr_2O_7$.
- (8) Determination of three dissociation constants of H₃PO₄ by pH-metric/potentiometric titration

V. Optical methods

- (1) Determination of pK of indicator by colorimetry.
- (2) To estimate the amount of NH₄Cl colorimetrically using Nesseler's Reagent.
- (3) To study the complex formation between Fe(III) and salicylic acid and find the formula and stability constant of the complex colorimetrically (Job's method).
- (4) To determine the dissociation constant of phenolphthalein colorimetrically.
- (5) Estimation of iron in wastewater sample using 1,10-phenanthroline.

(Note: One experiment from each section should be performed in the examination.)

Examination: CHE 206 Analytical Chemistry Laboratory (Lab 04)

| Time : 6-8 Hrs. (One day Examination) | | Total Marks : 100 |
|---------------------------------------|----------------------------|-------------------|
| А. | Exercise-I (Section A) | 20 |
| В. | Exercise-II (Section B) | 20 |
| C. | Viva (External + Internal) | 10 |
| Е. | Internal assessment* | 50 |
| | Total | 100 |

*- Internal assessment will be continuous and based on the performance of a student throughout the session along with satisfactory submission of the term work

Course Material/Learning Resources:

- (1) Quantitative analysis: Day and Underwood (Prentice-Hall of India)
- (2) Vogel's Text Book of Quantitative Inorganic Analysis-Bassett, Denney, Jeffery and Mendham (ELBS)
- (3) Analytical Chemistry: Gary D. Christian (Wiley, India).
- (4) Instrumental Methods of Analysis: Willard, Merrit, Dean, Settle (CBS Publishers, Delhi, 1986)
- (5) Instrumental Methods of Chemical Analysis: Braun (Tata McGraw-Hill)
- (6) Advanced Analytical Chemistry: Meites and Thomas (McGraw-Hill)
- (7) Instrumental Methods of Analysis: G. Chatwal and S. Anand (Himalaya Publishing House)
- (8) Analytical Chemistry: Problems and Solution-S. M. Khopkar (New Age International Publication)
- (9) Basic Concepts in Analytical Chemistry: S. M. Khopkar (New Age International Publication)

(10) Advance Analytical Chemistry: Meites and Thomas: (Mc Graw Hill)

- (11) An Introduction to Separation Science: L. R. Shyder and C. H. Harvath (Wiley Interscience)
- (12) Fundamentals of Analytical Chemistry: S. A. Skoog and D. W. West

(13) Instrumental Methods of Chemical Analysis: G. W. Ewing