

## **Department of Chemistry**

The Department of Chemistry under the School of Physical and Chemical Sciences forms a key component of the university. The department is composed of dynamic faculty members, students and research scholars who are actively engaged in knowledge creation and dissemination at the frontiers of the Chemical Sciences. The discipline has an encompassing effect on the biological and physical sciences and therefore considered a central science. The department believes in interdisciplinary approach of learning and fosters a culture of excellence. Undergraduate and Post-graduate students of chemistry are nurtured and mentored well to compete at the national and international level (e.g. selection for the summer research fellowships of National Academies of Sciences, award at National Science Film Festival, JAM, UGC-CSIR NET, GATE and more...). The masters (M.Sc.) and doctoral (Ph.D.) programmes were started in 2018 and 2019, respectively. Although the department is relatively younger, it is scaling new heights with every passing year. Many of the alumni are now well-placed in different research and academic institutions of repute. Knowledge and skills in chemistry play a crucial role in finding the solutions to most of the challenges (eg. energy, disease, and environment) faced by the mankind today. We envisage producing globally competent chemists who can solve the pressing problems of the nation.

### **MSc. Programme in Chemistry**

The programme is for the students who have an interest in chemistry and a desire to explore the frontiers of science. This is a unique programme that combines core chemistry (Organic, Inorganic and Physical) with Nano Chemistry and Green Chemistry. Along with thorough grounding in chemistry, it equips the students with the knowledge and skills in the emerging interdisciplinary area of green nanotechnology which has now become a crucial requirement for the sustainable development globally. Computational Chemistry and Medicinal Chemistry have also been incorporated to equip the students better. The programme envisages creating good bench strength of future scientists who can solve a wide range of issues and contribute to the scientific advancement of the nation.

There is ample opportunities and employability for chemists having sound knowledge, analytical skills and hands-on training on sophisticated instruments. The chemical industry is India's one of the largest manufacturing sectors and plays an integral role in the country's economic development. The Indian chemical sector currently accounts for 13-14% of total exports. In terms of volume of production, it is the twelfth-largest in the world and the third-largest in Asia. Currently, the per capita consumption of products of the Indian chemical industry is one-tenth of the world average, which reflects the huge potential for further growth. The "Make in India" scheme has further given a fresh impetus to this sector. For sustainable, environment-friendly growth, the sector is looking for new technologies that incorporate green chemistry and nanotechnology, and there lies the exciting and excellent career opportunities for young chemists. Besides the chemical industry, the training imparted in the interdisciplinary area of green nanotechnology will also enable the students to diversify and join other sectors such as energy, photovoltaics, photonics, biosensing, and healthcare etc.

The curriculum has been designed to keep abreast with changing times. In the long run, the programme is likely to produce globally competent chemists with bright innovative ideas. By understanding the nuances of chemistry, these young scientists would be creating new tools, products and technologies to address some of the world's biggest challenges such as (just to name a few) clean affordable energy, biomedical devices and drugs for treating diseases, bio-sensing and environmental remediation etc.

- **DURATION OF THE PROGRAMME:** Four semesters, July – December (odd semesters) and January – May (even semesters).
- **ADMISSION PROCEDURE:** The admission to the course shall be through an entrance examination, Central University Common Entrance Test (CUCET-2023) to be conducted on all-India basis.
- **ELIGIBILITY OF THE CANDIDATES:**  
Candidates who have passed B.Sc. examination of any recognized university or its equivalent examination with minimum of 55% marks in aggregate (or in honours subject) (50% in the case of SC/ST students) and who have taken Chemistry (General/Honours) as one of the subjects at the third year of the B.Sc.
- **Credit System: Theory:** 01-hour lecture per week – 01 credit.  
**Experimental Chemistry & Computational Chemistry:** 02 hours – 01 credit
- **Distribution of Points:** Theory (T) = 100 points; Practical (P) = 100 points.

**Theory of each paper:** 100 points

Distribution of points (Theory):

**1A:** Continuous Assessment Test (CAT): 3 CATs will be conducted at regular intervals in the entire semester in during regular class hours to assess student's progress. Each CAT will carry 10 points.

Total  $3 \times 10 = 30$  Points.

**1B:** End-Term: 70 points.

**Experimental Chemistry Lab.: 100 points**

Distribution of points (Practical): Tentative

**1A:** Class Participation/involvement in experiment/cleanliness/skill: 10 points

**2B:** Distribution of points of Final Exam: (i) Exam: 40 points, (ii) Viva: 30 points, (iii) Overall record (Performance, write-up, and on-time submission throughout the semester): 20 points.]

- **Grading System:**

There will be 10-point Scale Grading System starting with 4 and ending at 10. There will be additional Grade 'F' with Grade Point 'Zero'. A student having received Grade 'F' in a course will have to reappear in the examination of the said course. The following grading system will be used:

| Letter Grade               | Numerical Grade Point | Class Interval (in %)   |
|----------------------------|-----------------------|-------------------------|
| O (Outstanding)            | 10                    | Above 90 and $\leq 100$ |
| A <sup>+</sup> (Excellent) | 9                     | Above 80 and $\leq 90$  |
| A (Very Good)              | 8                     | Above 70 and $\leq 80$  |
| B <sup>+</sup> (Good)      | 7                     | Above 60 and $\leq 70$  |
| B (Above Average)          | 6                     | Above 50 and $\leq 60$  |
| C (Average)                | 5                     | Above 45 and $\leq 50$  |
| P (Pass)                   | 4.5                   | 40 to 45                |
| F (Fail)                   | 0                     | < 40                    |
| Ab (Absent)                | 0                     | Absent                  |

*Note:*

- (i) F= Fail, and the students graded with 'F' in a Programme or Course shall be required to re-appear in the examination.
- (ii) The minimum qualifying points for a course shall be 4.5 (i.e., 'P' grade).
- (iii) The students shall have to qualify in the Continuous Internal Assessment and the End-Semester examinations taken together.

### Types of Courses

| Nature of Course |                                          | Course Code | Description of the course                                                                                                                                                                                                                                                                                                                         |
|------------------|------------------------------------------|-------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 1.               | Discipline Based Core Course             | <b>DC</b>   | This is the foundational course which is to be compulsory studied by a student as a core requirement of a programme in a said discipline of study at PG level. This also includes the introductory course on research methodology, dissertation writing, project work, field work, lab work related to the subject.                               |
| 2.               | Discipline Based Core Elective Course    | <b>DE</b>   | This is the elective foundational course, aimed to expand the understanding in a specific area and emerged from the foundational knowledge. The students have choice to choose the course from a basket of DE                                                                                                                                     |
| 3.               | Open Elective (Interdisciplinary) course | <b>OE</b>   | This is elective course, aimed to enable exposure to some other discipline or domain. The students have to choose the open elective course from the other departments.                                                                                                                                                                            |
| 4.               | Mandatory elective Non-Credit Course     | <b>ME</b>   | This is the value added course to promote multidisciplinary and holistic education among the students. The course is of non-credit nature but mandatory to the complete successfully for the award of the Master's degree.<br><br>The students have to choose the ME courses, equivalent to at least 02 credits, from a basket of offered course. |

| SEMESTER-I   |                                               |        |
|--------------|-----------------------------------------------|--------|
| Course Code  | Nature of the Course                          | Credit |
| DC           | Discipline Based Core Courses                 | 16     |
| OE           | Open Elective (Interdisciplinary) course      | 04     |
| ME           | None-Credit Course equivalent to 02 credits   | --     |
| Total        |                                               | 20     |
| SEMESTER-III |                                               |        |
| Course Code  | Nature of the Course                          | Credit |
| DC           | Discipline Based Core Courses                 | 08     |
| DC / DE      | Discipline Based Core / Core Elective Courses | 08     |
| OE           | Open Elective (Interdisciplinary) course      | 04     |
| ME           | None-Credit Course equivalent to 02 credits   | --     |
| Total        |                                               | 20     |

| SEMESTER-II                            |                                                                                   |        |
|----------------------------------------|-----------------------------------------------------------------------------------|--------|
| Course Code                            | Nature of the Course                                                              | Credit |
| DC                                     | Discipline Based Core Courses (including 04 credits course on vocational Studies) | 16     |
|                                        | Introductory Course on Research Methodology (04 Credits)                          |        |
| DC / DE                                | Discipline Based Core / Core Elective Courses                                     | 04     |
| ME                                     | None-Credit Course equivalent to 02 credits                                       | --     |
|                                        |                                                                                   | 20     |
| Exit option with Post Graduate Diploma |                                                                                   |        |
| SEMESTER-IV                            |                                                                                   |        |
| Course Code                            | Nature of the Course                                                              | Credit |
| DC                                     | Discipline Based Core Courses                                                     | 12     |
|                                        | Dissertation/ Project Work / Lab Work/ Field Work*                                |        |
| DC / DE                                | Discipline Based Core / Core Elective Courses                                     | 0      |
|                                        |                                                                                   |        |
| ME                                     | None-Credit Course equivalent to 02 credits                                       | --     |
| Total                                  |                                                                                   | 20     |

### Salient features of the programme

- Nano Chemistry, Medicinal Chemistry, Green Chemistry and Green Energy systems have been incorporated in the curriculum to develop a thorough understanding of these emerging fields and their relevance in the daily life of mankind.
- Computational Chemistry, theory and labs, have also been made part of the curriculum to make the students proficient in theoretical modelling and simulations.
- Besides imparting in-depth knowledge, hands-on training will also be given to students on sophisticated instruments which are a prerequisite for being employable in industries and succeeding in cutting-edge research.
- For proper utilization of the summer break period, students will be encouraged to take up a summer activity. This activity may include research internships in academic/research institutions or industrial labs. It may also include activities related to science communication such as writing a popular science article in a magazine or writing a review article in a scientific journal. It also includes activities such as science film making etc. The summer project should be done at the end of 2<sup>nd</sup> Semester during the summer break period.
- Students from both PCB and PCM streams can join this degree programme. We believe that knowledge of both mathematics and biology is necessary to understand the nuances of chemistry.
- The M.Sc. Programme in Chemistry follows CBCS approach.
  - A minimum of 80 credits must be completed by the students during the entire programme. However, students can earn more credits by opting for additional courses from the elective baskets.

- Out of the 80 credits a total of 56 credits should be earned through core courses. For semester 1<sup>st</sup> and 3<sup>rd</sup>, students have to choose courses from the odd semester courses list. Similarly, for semester 2<sup>nd</sup> and 4<sup>th</sup>, students have to choose courses from even semester courses list.
- Out of the 80 credits a total of 24 credits should be earned through electives following cafeteria model under CBCS scheme. Out of 24 credits, 8 credits (two courses) should be earned through open elective interdisciplinary courses (OE) offered by other departments/centers /SWAYAM.
- Students can opt for the courses from SWAYAM portal in consultation with the faculty members/mentors of the department.
- The department will announce in advance about the elective courses, DE and OE, to be run in the coming semester.
- Along with the requisite core/and elective courses, the students must select two Mandatory Elective Non-Credit course (ME) in two semesters. For ME courses, the students will not get any kind credit score; only a certificate of satisfactory completion will be issued. These courses can be selected from the basket of ME courses offered by the department of chemistry or other department of the university or SWAYAM portal.
- Core and elective courses of the department are of 4 credits each.
- Students will not be allowed to repeat the elective courses during the programme.
- *Out of elective courses offered, only few selected ones will be floated in a particular academic session and at least a certain number (to be decided by the departmental committee) of total students enrolled must opt for a particular elective paper to run that course.*
- Allotment of different branches of specialization will be done at the end of second semester. An order of preference must be submitted by each student for the three different specializations. Based on the two parameters, the choice and performance upto 2<sup>nd</sup> semester, the specialization will be allotted subject to maximum of 40% of total strength of students in one specialization.

### **FIRST SEMESTER (ODD SEMESTER)**

| Paper Code                                     | Course Title                                                                       | Theory/<br>Practical<br>(Hrs/Week) | Total<br>Marks | Credits  |          |          |
|------------------------------------------------|------------------------------------------------------------------------------------|------------------------------------|----------------|----------|----------|----------|
|                                                |                                                                                    |                                    |                | L        | T        | P        |
|                                                | <b>Semester I</b>                                                                  |                                    |                |          |          |          |
| <b>CHE81DC01004</b>                            | Advanced Inorganic Chemistry-I                                                     | <b>4</b>                           | <b>100</b>     | <b>3</b> | <b>1</b> | <b>0</b> |
| <b>CHE81DC02004</b>                            | Advanced Organic Chemistry-I                                                       | <b>4</b>                           | <b>100</b>     | <b>3</b> | <b>1</b> | <b>0</b> |
| <b>CHE81DC03004</b>                            | Advanced Physical Chemistry-I                                                      | <b>4</b>                           | <b>100</b>     | <b>3</b> | <b>1</b> | <b>0</b> |
| <b>CHE81DC01104</b>                            | Inorganic Chemistry Lab<br>(Vocational Course)                                     | <b>8</b>                           | <b>100</b>     | <b>0</b> | <b>0</b> | <b>4</b> |
| <b>CHE81OE - - - 04 /<br/>CHE81SW - - - 04</b> | <b>Open Elective (Inter-School or<br/>Inter Department or SWAYAM<br/>elective)</b> | <b>4</b>                           | <b>100</b>     | <b>4</b> | <b>0</b> | <b>0</b> |
| <b>CHE81ME00100</b>                            | <b>Need To choose from the Given</b>                                               | <b>2</b>                           | <b>50</b>      | <b>0</b> | <b>0</b> | <b>0</b> |

|                                                |                |  |  |           |  |  |
|------------------------------------------------|----------------|--|--|-----------|--|--|
|                                                | <b>basket*</b> |  |  |           |  |  |
| <b>Minimum Credits required for Semester I</b> |                |  |  | <b>20</b> |  |  |

### **SECOND SEMESTER (EVEN SEMESTER)**

| Paper Code                                      | Course Title                                                    | Theory/<br>Practical<br>(Hrs/Week) | Total<br>Marks | Credits   |          |          |
|-------------------------------------------------|-----------------------------------------------------------------|------------------------------------|----------------|-----------|----------|----------|
|                                                 |                                                                 |                                    |                | L         | T        | P        |
|                                                 | <b>Semester II</b>                                              |                                    |                |           |          |          |
| <b>CHE82DC01204</b>                             | Photochemical and magnetic properties of complexes              | <b>4</b>                           | <b>100</b>     | <b>3</b>  | <b>1</b> | <b>0</b> |
| <b>CHE82DC02204</b>                             | Reaction Mechanism (II), Pericyclic and Photochemical Reactions | <b>4</b>                           | <b>100</b>     | <b>3</b>  | <b>1</b> | <b>0</b> |
| <b>CHE82DC03204</b>                             | Quantum Chemistry                                               | <b>4</b>                           | <b>100</b>     | <b>3</b>  | <b>1</b> | <b>0</b> |
| <b>CHE82DC04004</b>                             | Research Methodology                                            | <b>4</b>                           | <b>100</b>     | <b>3</b>  | <b>1</b> | <b>0</b> |
| <b>CHE82DC03104</b>                             | Physical Chemistry Lab<br>(Vocational Course)                   | <b>8</b>                           | <b>100</b>     | <b>0</b>  | <b>0</b> | <b>4</b> |
| <b>CHE82ME00200</b>                             | <b>Need To choose from the Given basket*</b>                    | <b>2</b>                           | <b>50</b>      | <b>0</b>  | <b>0</b> | <b>0</b> |
| <b>Minimum Credits required for Semester II</b> |                                                                 |                                    |                | <b>20</b> |          |          |

### **THIRD SEMESTER (ODD SEMESTER)**

| Paper Code          | Course Title                                                                     | Theory/<br>Practical<br>(Hrs/Week) | Total<br>Marks | Credits  |          |          |
|---------------------|----------------------------------------------------------------------------------|------------------------------------|----------------|----------|----------|----------|
|                     |                                                                                  |                                    |                | L        | T        | P        |
|                     | <b>Semester III</b>                                                              |                                    |                |          |          |          |
| <b>CHE91DC02104</b> | Organic Chemistry Lab<br>(Vocational Course)                                     | <b>8</b>                           | <b>100</b>     | <b>0</b> | <b>0</b> | <b>4</b> |
| <b>CHE91DC03304</b> | Molecular Spectroscopy                                                           | <b>4</b>                           | <b>100</b>     | <b>3</b> | <b>1</b> | <b>0</b> |
| <b>DC/ DE</b>       | <b>Organic/ Inorganic/Physical Specialization Paper* (any one)</b>               |                                    |                |          |          |          |
| <b>CHE91DC01304</b> | Inorganic Materials and their applications                                       | <b>4</b>                           | <b>100</b>     | <b>3</b> | <b>1</b> | <b>0</b> |
| <b>CHE91DC02304</b> | Modern Organic Synthesis                                                         | <b>4</b>                           | <b>100</b>     | <b>3</b> | <b>1</b> | <b>0</b> |
| <b>CHE91DC03404</b> | Applied Electrochemistry                                                         | <b>4</b>                           | <b>100</b>     | <b>3</b> | <b>1</b> | <b>0</b> |
| <b>DC/ DE</b>       | <b>Organic/ Inorganic/Physical Specialization Paper* (any one)</b>               |                                    |                |          |          |          |
| <b>CHE91DC01404</b> | Inorganic Reaction Mechanism, Organometallics and Advance Bioinorganic Chemistry | <b>4</b>                           | <b>100</b>     | <b>3</b> | <b>1</b> | <b>0</b> |
| <b>CHE91DC02404</b> | Chemistry of Biomolecules                                                        | <b>4</b>                           | <b>100</b>     | <b>3</b> | <b>1</b> | <b>0</b> |

|                                                  |                                                                                    |          |            |           |          |          |
|--------------------------------------------------|------------------------------------------------------------------------------------|----------|------------|-----------|----------|----------|
| <b>CHE91DC03504</b>                              | Advanced Photochemistry                                                            | <b>4</b> | <b>100</b> | <b>3</b>  | <b>1</b> | <b>0</b> |
| <b>CHE91OE---04 /<br/>CHE81SW---04</b>           | <b>Open Elective<br/>(Inter-School or Inter-Department<br/>or SWAYAM elective)</b> | <b>4</b> | <b>100</b> | <b>4</b>  | <b>0</b> | <b>0</b> |
| <b>ME</b>                                        | <b>Need To choose from the Given<br/>basket*</b>                                   | <b>2</b> | <b>50</b>  | <b>0</b>  | <b>0</b> | <b>0</b> |
| <b>Minimum Credits required for Semester III</b> |                                                                                    |          |            | <b>20</b> |          |          |

#### **FOURTH SEMESTER (EVEN SEMESTER)**

| <b>Paper Code</b>   | <b>Course Title</b>                                        | <b>Theory/<br/>Practical<br/>(Hrs/Week)</b> | <b>Total<br/>Marks</b> | <b>Credits</b> |          |          |
|---------------------|------------------------------------------------------------|---------------------------------------------|------------------------|----------------|----------|----------|
|                     |                                                            |                                             |                        | <b>L</b>       | <b>T</b> | <b>P</b> |
|                     | <b>Semester IV</b>                                         |                                             |                        |                |          |          |
| <b>CHE92DC03604</b> | Surface Phenomena, Colloids and Statistical Thermodynamics | <b>4</b>                                    | <b>100</b>             | <b>3</b>       | <b>1</b> | <b>0</b> |
| <b>CHE92DC05108</b> | Scientific literature Survey and Dissertation Work*        | <b>16</b>                                   | <b>200</b>             | <b>2</b>       | <b>0</b> | <b>6</b> |

**or**

|                                                 |                                                                   |            |            |           |          |          |
|-------------------------------------------------|-------------------------------------------------------------------|------------|------------|-----------|----------|----------|
| <b>CHE92DC06104</b>                             | Scientific literature Survey and Scientific Activities            | <b>4+4</b> | <b>100</b> | <b>2</b>  | <b>0</b> | <b>2</b> |
| <b>CHE92DC07004</b>                             | Chemical Education                                                | <b>4</b>   | <b>100</b> | <b>3</b>  | <b>1</b> | <b>0</b> |
| <b>DC /DE</b>                                   | <b>Organic/ Inorganic/Physical Specialization Paper*(any one)</b> |            |            |           |          |          |
| <b>CHE92DC01504</b>                             | Chemistry of Materials                                            | <b>4</b>   | <b>100</b> | <b>3</b>  | <b>1</b> | <b>0</b> |
| <b>CHE92DC02504</b>                             | Advanced Medicinal Chemistry                                      | <b>4</b>   | <b>100</b> | <b>3</b>  | <b>1</b> | <b>0</b> |
| <b>CHE92DC03704</b>                             | Advanced Quantum Mechanics and Surface Chemistry                  | <b>4</b>   | <b>100</b> | <b>3</b>  | <b>1</b> | <b>0</b> |
| <b>DC/ DE</b>                                   | <b>Organic/ Inorganic/Physical Specialization Paper*(any one)</b> |            |            |           |          |          |
| <b>CHE92DC01604</b>                             | Applications of spectroscopy techniques to inorganic systems      | <b>4</b>   | <b>100</b> | <b>3</b>  | <b>1</b> | <b>0</b> |
| <b>CHE92DC02604</b>                             | Spectroscopy and Chiroptical properties                           | <b>4</b>   | <b>100</b> | <b>3</b>  | <b>1</b> | <b>0</b> |
| <b>CHE92DC03804</b>                             | Lasers in Chemistry                                               | <b>4</b>   | <b>100</b> | <b>3</b>  | <b>1</b> | <b>0</b> |
| <b>ME</b>                                       | <b>Need To choose from the Given<br/>basket*</b>                  | <b>2</b>   | <b>50</b>  | <b>0</b>  | <b>0</b> | <b>0</b> |
| <b>Minimum Credits required for Semester IV</b> |                                                                   |            |            | <b>20</b> |          |          |

**\*Note:**

1. Based on the choice and performance up to the second semester, students will be assigned projects under the supervision of various faculty members at the start of semester III.
2. The students will be required to carry out a thorough literature survey on the assigned topic and submit the report at the end of semester-III (equivalent to 2 Credits to be assigned at the end of semester-IV) and propose a research plan for the project work to be conducted in semester IV.
3. Based on the project work done in semester-IV, students will write and submit the dissertation. Evaluation will be done based on report submissions, presentations and open viva-voce examination which will be conducted at the end of semester-IV. The total of 8 credits will be assigned to the students for the entire course (2 for Sci. Lit. survey + 6 for Dissertation work).

**#Note:**

- (i) Students can choose any two courses from the MENC basket of any department/school of the university or the SWAYAM portal.
- (ii) The MENC basket of the Department of Chemistry is given below.

### **ELECTIVES COURSES**

**For DE/OE**

| <b>Code No</b>           | <b>Title</b>                                      | <b>Theory/Practical<br/>(Hrs/Week)</b> | <b>Credits<br/>L/T/P</b> |
|--------------------------|---------------------------------------------------|----------------------------------------|--------------------------|
| <b>DE01004/ OE01004</b>  | Basics of Supramolecules and its advancement      | <b>4</b>                               | <b>3/1/0</b>             |
| <b>DE02004 / OE02004</b> | Green Chemistry I: Solvents & Synthesis           | <b>4</b>                               | <b>3/1/0</b>             |
| <b>DE03004 / OE03004</b> | Solid State and Structural Chemistry              | <b>4</b>                               | <b>3/1/0</b>             |
| <b>DE03104 / OE03104</b> | Advanced Instrumental Techniques-I                | <b>4</b>                               | <b>3/1/0</b>             |
| <b>DE02104 / OE02104</b> | Green Chemistry II: Catalysis                     | <b>4</b>                               | <b>3/1/0</b>             |
| <b>DE02204 / OE02204</b> | Nucleoside, Advances in Nucleic Acid and Proteins | <b>4</b>                               | <b>3/1/0</b>             |
| <b>DE02304 / OE02304</b> | Chemistry of Natural Products                     | <b>4</b>                               | <b>3/1/0</b>             |
| <b>DE02404 / OE02404</b> | Agrochemicals                                     | <b>4</b>                               | <b>3/1/0</b>             |
| <b>DE03204 / OE03204</b> | Nano Chemistry                                    | <b>4</b>                               | <b>3/1/0</b>             |
| <b>DE03304 / OE03304</b> | Advanced Instrumental Techniques-II               | <b>4</b>                               | <b>3/1/0</b>             |
| <b>DE02504 / OE02504</b> | Green Energy Systems                              | <b>4</b>                               | <b>3/1/0</b>             |
| <b>DE03402 / OE03402</b> | Fundamentals of Nuclear Chemistry                 | <b>2</b>                               | <b>2/0/0</b>             |



**ME Non-Credit Course**

| Code No                             | Title                                                               | Theory/Practical (Hrs/Week) | Total Marks | Credits |
|-------------------------------------|---------------------------------------------------------------------|-----------------------------|-------------|---------|
| ME00100                             | Contributions of Ancient, Medieval and Contemporary Indian Chemists | 2                           | No Grading  | 0       |
| ME00200                             | Science Communication                                               | 2                           | No Grading  | 0       |
| <b>ME Course on SWAYAM Platform</b> |                                                                     |                             |             |         |
| ME<br>ME00200                       | Academic writing<br>(H.N.B. Garwhal University, Dr. Ajay Semalty)   |                             | 12 Weeks    | 0       |

**SWAYAM COURSES (OEIC)****Approved by Department of Chemistry\***

| SN | Code No | Swayam Course                                             | Course Offered By                                   | Course Duration |
|----|---------|-----------------------------------------------------------|-----------------------------------------------------|-----------------|
| 1. | SW01004 | Transition metal organometallics in catalysis and biology | IIT Bombay<br>Prof. P. Ghosh                        | 12 Weeks        |
| 2. | SW02004 | Medicinal Chemistry                                       | IISER Pune<br>Prof. Harinath Chakrapani             | 12 Weeks        |
| 3. | SW03004 | Molecular Spectroscopy                                    | IIT Bombay<br>Prof. Anindya Datta                   | 12 Weeks        |
| 4. | SW01104 | Industrial Inorganic Chemistry                            | Prof. Debashis Ray<br>IIT Kharagpur                 | 12 Weeks        |
| 5. | SW02104 | Essential of biomolecules Nucleic Acid and Peptides       | Prof. Lal Mohan Kundu IIT Guwahati                  | 12 Weeks        |
| 6. | SW02204 | Biochemistry                                              | Prof. Swagata Dasgupta IIT Kharagpur                | 12 Weeks        |
| 7. | SW01204 | Chemistry of Main Group Elements                          | Prof. M. S. Balakrishna<br>IIT Bombay               | 12 Weeks        |
| 8. | SW02304 | Biomass Characterization                                  | Prof. K. Arun Kumar<br>Central University of Kerala | 12 Weeks        |
| 9. | SW02404 | Reagents in Organic Synthesis                             | IIT Guwahati<br>Prof. Subhas Chandra Pan            | 12 Weeks        |

|     |         |                                          |                                                  |          |
|-----|---------|------------------------------------------|--------------------------------------------------|----------|
| 10. | SW02504 | Principles of Organic Synthesis          | IIT Guwahati<br>Prof. T. Punniyamurthy           | 12 Weeks |
| 11. | SW03104 | Chemical Crystallography                 | IISER Mohali<br>Prof. Angshuman Roy<br>Choudhury | 12 Weeks |
| 12. | SW01304 | Biological Inorganic Chemistry           | Prof. Debashis Ray<br>IIT Kharagpur              | 12 Weeks |
| 13. | SW02504 | Drug Delivery: Principle and Engineering | Prof. Rachit Agarwal<br>IISc Bangalore           | 12 Weeks |
| 14. | SW03204 | Analytical Chemistry                     | Prof. Debashis Ray<br>IIT Kharagpur              | 12 Weeks |
| 15. | SW03304 | Biophysical Chemistry                    | Prof. Pramit K Chowdhury,<br>IIT-Delhi           | 12 Weeks |

\*The list is dynamic one and is revised every semester by the departmental committee which may involve addition/deletion of a few courses depending on their availability and suitability to our academic programme

### **FIRST SEMESTER (ODD SEMESTER)**

| <b>Course Title: Advanced Inorganic Chemistry-I</b> |                                                                          |                        |                          |
|-----------------------------------------------------|--------------------------------------------------------------------------|------------------------|--------------------------|
| <b>Course Code</b>                                  | <b>CHE81DC01004</b>                                                      | <b>Credits</b>         | 4                        |
| <b>L + T + P</b>                                    | 3 + 1 + 0                                                                | <b>Course Duration</b> | One Semester             |
| <b>Semester</b>                                     | Odd                                                                      | <b>Contact Hours</b>   | 45 (L) + 15 (T)<br>Hours |
| <b>Methods of Content Interaction</b>               | Lecture, Tutorials, Group discussion; self-study, seminar, presentations |                        |                          |
| <b>Assessment and Evaluation</b>                    | Lecture, Tutorials, Group discussion; self-study, seminar, presentations |                        |                          |

#### **Course Objectives**

- To develop understanding of group theory and apply the concepts of symmetry to molecular systems
- To enhance the understanding of ionic and covalent bonding in view of point groups and molecular symmetry.
- To impart in-depth knowledge about metal-ligand equilibrium reactions
- To equip the students with necessary skills to determine the equilibrium constants using various instrumental techniques

**Learning Outcomes:** After completion of the course the learners will be able to:

- Identify the symmetry elements present in a molecule,
- Assign the point groups to a molecule and perform symmetry operations
- Analyse the molecular structure and bonding in molecules and coordination complexes with the help of group theory

- Determine the overall and stepwise formation constants of metal-complexes

### UNIT-I

**Chemical Bonding:** VSEPR model, shapes of molecules- $\text{ClF}_3$ ,  $\text{ICl}_4^-$ ,  $\text{TeF}_5^-$ ,  $\text{I}_3^-$ ,  $\text{TeCl}_6^{2-}$ ,  $\text{XeF}_6$ ,  $\text{SbCl}_6^{3-}$ ,  $\text{IF}_7$ ,  $\text{ReF}_7$ ,  $\text{XeF}_8^{2-}$ ,  $\text{TaF}_8^{3-}$ , Bent rules and energetics of hybridization; electronegativity and partial ionic character; Bonds-Multicenter bonding.

Lattice energy: Born-Landé equation, Kapustinskii equation; polarizability and partial covalent character, radius-ratio rules, structures of simple solids, Zintl-isoelectronic relationship in solids. Molecular orbital theory: LCAO and MO diagrams of heteronuclear diatomic ( $\text{CO}$ ,  $\text{NO}$ ,  $\text{HF}$ ,  $\text{ICl}$ ) and triatomic molecules ( $\text{CO}_2$  and  $\text{NO}_2^-$ ).

### UNIT-II

**Metal-ligand bonding-** Crystal field theory, salient features, spectrochemical series, splitting of d-orbitals in tetragonal, square planar, trigonal bipyramidal and square-pyramidal geometry, applications of CFT-colours of transition metal complexes, magnetic properties of octahedral complex, distortion of octahedral complex, CFSE and their uses, factors affecting CFSE, limitations of CFT, experimental evidence for metal-ligand covalent bonding in complexes, nephelauxetic effect, Ligand Field Theory, MO theory: tetrahedral and octahedral complexes (including  $\pi$ -bonding), angular overlap model. Stereochemical non-rigidity, self-assembly in supramolecular chemistry.

Bonding in metal clusters: M-M bond and metal atom clusters, carbonyl and halide clusters, bonding in  $[\text{ReCl}_8]^{2-}$ . Metal carbonyl clusters- LNCC's and HNCC's. Electron counting in carbonyl clusters.

### UNIT-III

**Metal-Ligand equilibria in solution-** Step-wise and over all formation constant and their relationship, trends in step-wise constant, kinetic and thermodynamic stability of metal complexes, factors affecting the stability of metal complexes with reference to the nature of the metal ion and ligand, chelate effect, macrocyclic effect and their thermodynamic origin. Determination of binary formation constant by pH-metry, spectrophotometry, polarography and ion exchange methods.

**Structure and bonding-** Structure and bonding in isocyanide,  $\text{CO}$ ,  $\text{NO}$ ,  $\text{N}_2$  tertiary phosphine and other similar ligands and their transition metal complexes.

**Stereoisomerism-** Chirality, optical activity and isomerism in inorganic complexes.

### UNIT-IV

**Symmetry and Group Theory in Chemistry:** Definition of groups, subgroups, cyclic groups, conjugates relationships, classes, simple theorems in group theory. Symmetry elements and symmetry operations, point groups, Schönflies notations, representations of groups by matrices, reducible and irreducible representations, characters of representations, Great Orthogonality Theorem (without proof) and its applications, character tables and their uses (representations for the  $C_n$ ,  $C_{nv}$ ,  $C_{nh}$ ,  $D_{nh}$  etc groups to be worked out explicitly), Mulliken symbols for irreducible representations Direct products.

### SUGGESTED TEXT BOOKS

1. Basic Inorganic Chemistry-F.A.Cotton, G.Wilkinson and P.L.Gaus; John Wiley and sons. Inc, 6<sup>th</sup> edition.
2. Inorganic Chemistry; J. E.Huheey, E.A. Keiter and R. L. Keiter, Addison; Wesley.
3. Inorganic Chemistry, D. F. Shriver, P.W.Atkins and C. H. Langford, ELBS; Oxford University Press.
4. Concise Inorganic Chemistry, 5<sup>th</sup> edition; J. D. Lee (1996).
5. Chemical Applications of Group Theory, F. A. Cotton, Wiley Eastern (1976).

### SUGGESTED REFERENCE BOOKS

1. Basic Organometallic Chemistry: Concepts, Syntheses and Applications of Transition metals, 2010, CRC Press and Universities Press.
2. Advanced Inorganic Chemistry, 6<sup>th</sup> edition; F. A. Cotton and G. Wilkinson.
3. Inorganic Chemistry, 3<sup>rd</sup> Edition; Gary.L. Miessler and Donald. A. Tarr (2007).
4. Molecular Symmetry, D.S. Schonland, Van Nostrand (1965).
5. Chemistry of Elements; N. N.Greenwood and A. E. Earnshaw, Butterworth Heinemann (1997).

| Course Title: Advanced Organic Chemistry-I |                                                                          |                 |                       |
|--------------------------------------------|--------------------------------------------------------------------------|-----------------|-----------------------|
| Course Code                                | CHE81DC02004                                                             | Credits         | 4                     |
| L + T + P                                  | 3 + 1+ 0                                                                 | Course Duration | One Semester          |
| Semester                                   | Odd                                                                      | Contact Hours   | 45 (L) + 15 (T) Hours |
| Methods of Content Interaction             | Lecture, Tutorials, Group discussion; self-study, seminar, presentations |                 |                       |

**Course Objectives:** To learn the basic and advanced concepts of chemical bonding, reaction mechanisms, and prediction of reaction mechanisms by the physical phenomenon. Develop knowledge in-depth about stereochemistry, and applications of organometallic compounds in organic synthesis.

#### Learning Outcomes:

- Students will be able to make the correlation of bonding, structure, reactivity, and stability of organic molecules. And by using the above concepts, students will be able to understand the spatial arrangements of substituents in organic molecules and their implication in stereoselective reactions.
- Depth knowledge of different kinds of reaction mechanism and also know different tools available to predict the reaction mechanism.
- Students will be able to develop a basic knowledge of Organometallic compounds and their application in organic synthesis.

- Understand and apply the applications of organometallic compounds for catalytic applications, in the construction of C-C, C-C multiple bonds, C=X, and C-X bonds which is relevant to pharmaceutical and industrial applications.

### UNIT-I

**Physical Organic Chemistry:** Molecular Orbital Theory, Thermodynamic and kinetic control reactions, Thermodynamic Properties, Reaction Kinetics, Interpretation of rate constant, Hammond postulate, Curtin-Hammett principle. Potential energy diagrams, transition states and intermediates.

**Methods of determining mechanisms:** Based on the structure of products, determination of the presence of intermediates, isotopic labelling, isotope effects, chemical trapping and crossover experiments. Use of IR and NMR in the investigation of reaction mechanisms.

### UNIT-II

**Stereochemistry:** Chirality in compounds with a stereogenic centre, Stereogenic unit: Center of chirality, axis of chirality, plane of chirality and helicity. Stereochemistry of allenes, alkylidene, biphenyls, cyclophanes, and Ansa compounds, *trans*-cyclooctene, helicenes, and spiranes (with a stereogenic axis).

**Conformational analysis:** Conformational analysis of cycloalkanes: cyclobutane, cyclopentane, cyclohexanes (monosubstituted e.g., methyl, iso-propyl, tert-butyl and disubstituted cyclohexanes e.g., dialkyl, dihalo, diols) and cycloheptane.

Nomenclature and conformations of fused rings e.g. indane, decalines and perhydrophenanthrene, bridged ring systems like bicyclo[2.2.2], [2.2.1] systems.

**Dynamic Stereochemistry:** Fundamental of asymmetric synthesis: Introduction, Topocity in molecules Homotopic, stereoheterotopic (enantiotopic and diastereotopic), groups and face asymmetry, Cram's and Prelog's rules substitution and addition criteria. Prochirality nomenclature: Pro-R, Pro-S, Re and Si. Selectivity in synthesis: stereo specific reaction, stereo selective reactions-examples of addition, elimination, substitution and rearrangement reactions. Enantioselectivity and diastereoselectivity.

### UNIT-III

**Addition Reactions: Addition to carbon – carbon multiple bonds:** Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals. Regio, stereo- and chemoselectivities. Cis and trans additions. Orientation and reactivity. Addition to cyclopropane ring. Additions to C=C double bonds that are related to cycloadditions and form three-membered rings. Hydrogenation of double and triple bonds, hydrogenation of aromatic rings. Addition of alkenes and/or alkynes to alkenes and / or alkynes. Ene synthesis. Michael reaction.

**Methods for forming Carbon-carbon multiple bonds: Elimination Reactions:** The E<sub>2</sub>, E<sub>1</sub> and E<sub>1cB</sub> mechanisms. Orientation of the double bond. Reactivity- effects of substrate structure, attacking the base, the leaving group and the medium. Mechanism and orientation in pyrolytic elimination reactions (including Chugaev reaction), stabilized and unstabilized Wittig reagents, and olefination reactions.

### UNIT-IV

**Basic principles, preparation, properties, and applications of Organometallic in Organic Synthesis:**

Preparation and applications of Grignard, lithium organocuprates / Organocopper reagents in organic synthesis.

**Organosilicons:** Introduction, preparation, and general applications in organic synthesis, reactions involving  $\beta$ -carbocations and  $\alpha$ -carbanions, the utility of trimethyl silyl halides, cyanides, and triflates

Applications of Pd/Ni/Zn/Mo/W Complexes in organic synthesis: Baylis-Hillman reaction, Kulinkovich reaction, Sakurai reaction, Ugi reaction. Brook rearrangement; Tebbe olefination. Metal mediated C-C and C-X coupling reactions: Heck, Stille, Suzuki, Stille coupling, Kumada coupling, Negishi and Sonogashira, Nozaki-Hiyama, Buchwald-Hartwig, Ullmann coupling reactions, directed ortho metalation, Pauson Khand reaction, synthesis and use of Zinc dialkyls, olefin-cross metathesis/ring-closing metathesis reactions, Simmons Smith, and Reformansky reaction.

### SUGGESTED TEXT BOOKS

1. Advanced Organic Chemistry–Reactions, Mechanism and Structure, Jerry March, John Wiley (2008).
2. Advanced Organic Chemistry, F.A. Carey and R. J. Part A, Sundberg Springer; 5<sup>th</sup> Corrected ed. 2007
3. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman, (2000).
4. Organic Chemistry, R. T. Morrison and R N Boyd, Prentice-Hall, (1998).
5. Principles of Organic Synthesis, R.O. C. Norman and J.M. Coxon, Blackie Academic and Professional, (1996).
6. Stereochemistry of Organic Compounds, D. Nasipuri, New-Age International, (1999).
7. Smith M. B. and March J. March's Advanced Organic Chemistry, Wiley.
8. Carey F. A. and Sundberg R. Advanced Organic Chemistry, Part B, Plenum Press.
9. Norman R. O. C. and Coxon J. M. Principles of Organic Synthesis, Nelson Thornes

### SUGGESTED REFERENCE BOOK

1. Mechanism and Theory in Organic Chemistry, T. H. Lowry and K. S. Richardson, Addison-Wesley, 1998.
2. Structure and mechanism of Organic Chemistry, C. K. Ingold, Cornell University Press (1999).
3. Stereochemistry of Carbon Compounds, E.L.Eliel, S. H. Wilen and L. N. Mander, John Wiley,(1994).
4. Organic Chemistry, Volumes I and II, I LFinar, Longman,(1999).
5. Hegedus, L.S.; Transition metals in the synthesis of complex organic molecules, second edition, University Science, Book, CA, 1999.
6. Trost B. M. and Fleming I. Comprehensive Organic Synthesis, Pergamon Press.
7. László Kürti and Barbara Czákó:, Strategic Applications of Named Reactions in Organic Synthesis, Elsevier Academic, Burlington, 2005.

8. Schlosser, M., Organometallics in Synthesis, A manual, John Wiley, New York, 1996.
9. Handbooks of reagents for organic synthesis by Reich and Rigby, Vol-I-IV.
10. Astruc, D.; Organometallic Chemistry and Catalysis, Springer Verlag, 2007.
11. Davies, S. G.; Organotransition metal chemistry: Applications to organic synthesis, Pergamon Press, New York, 1986.

| <b>Course Title: Advanced Physical Chemistry-I</b> |                                                                          |                        |                          |
|----------------------------------------------------|--------------------------------------------------------------------------|------------------------|--------------------------|
| <b>Course Code</b>                                 | <b>CHE81DC03004</b>                                                      | <b>Credits</b>         | 4                        |
| <b>L + T + P</b>                                   | 3 + 1 + 0                                                                | <b>Course Duration</b> | One Semester             |
| <b>Semester</b>                                    | Odd                                                                      | <b>Contact Hours</b>   | 45 (L) + 15 (T)<br>Hours |
| <b>Methods of Content Interaction</b>              | Lecture, Tutorials, Group discussion; self-study, seminar, presentations |                        |                          |

#### **Course Objectives:**

- To develop an understanding of thermodynamics and apply the concepts to various physicochemical processes and systems
- To equip the students with necessary skills to analyse physicochemical changes with the help of phase diagrams
- To develop understanding of chemical kinetics
- To acquaint the students with the core concepts of electrochemistry

**Learning Outcomes:** After completion of the course the learners will be able to:

- Explain physicochemical changes with the help of phase diagrams
- Find out the rate and order of reactions
- Use electrochemical techniques for estimation of metal ions and biologically relevant
- Design a photoelectrochemical cell

### **UNIT-I**

#### **Thermodynamics-I**

**Thermodynamics:** Concepts of partial molar properties—partial molar free energy, chemical potential, partial molar volume and its significance. Gibbs-Duhem equation, Gibbs-Duhem-Margulus equation. Determination of partial molar volume: Graphical method, intercept method and apparent molar volume method. Concept of fugacity; Determination of fugacity by graphical method and compressibility factor method. Activity and activity coefficient: Determination of activity coefficient by EMF and solubility method. Thermodynamics of non-ideal system-Excess thermodynamic function,  $G^E$ ,  $S^E$ ,  $H^E$  etc.

**Phase Rule:** Derivation of phase rule from the concept of chemical potential. Application of Phase Rule to three components system: Principle of triangular diagram: Plots for a mixture of three liquids consisting of one, two and three pairs of partially miscible liquids.

## UNIT-II

**Reaction Dynamics-I:** Macroscopic and microscopic kinetics, Review of theories of reaction kinetics, Collision theory and Transition state theory, Comparison of collision theory with transition state theory, Arrhenious equation- characteristics, Significance of energy of activation, Temperature coefficient and its evaluation. Thermodynamical formulation of reaction rates (Wyne-jonesand Eyring treatment), Reaction between ions in solutions– Influence of ionic strength on reaction rates (primary and secondary salt effects).

Concept of Steady state kinetics, Chain reactions–chain length and chain inhibition, comparison of photochemical and thermal reactions, Mechanisms of thermal and photochemical reactions between hydrogen-bromine and hydrogen-chlorine. Comparative study of thermal and photochemical hydrogen-halogen reactions. Pyrolysis of acetaldehyde, Decomposition of ethane.

## UNIT-III

**Catalysis:** Kinetics of homogeneous catalysis-kinetics of auto catalytic reactions, kinetics of acid-base catalysed reactions. Comparison of enzyme catalysed and chemical catalyse dreactions, Mechanism (Lock and Key theory), Kinetics of enzyme catalyzed reactions– Henri-Michaelis- Menten mechanism, Significance of Michaelis-Menten constant, Lineweaver-Burk plot. Effects of enzyme concentration, pH, Temperature, Activators and Inhibitors on enzyme activity. Theories of unimoleuclar reactions.

## UNIT-IV

### Electrochemistry-I

**Electrochemistry of solutions:** Ionic atmosphere, Debye-Huckel theory for the problem of activity coefficient, Debye-Huckel limiting Law, its modification for finite size of ions and for appreciable concentration, Debye-Hückel-Onsagar conductance equation and its extension to short-range ion-ion interaction leading to ion pair formation (Fuss modification). Bjerrum's model for pair-wise ionic association, Ion association, triple-ion pairs, and conductance minima. Thermodynamics of electrified interface, derivation of electro-capillary Lipmann's equation, surface excess, thermodynamic aspects of surface excess. The method of determination and measurement of interfacial tension as a function of applied potential difference across the interface.

### SUGGESTED TEXT BOOKS

1. Physical Chemistry: A Molecular Approach, McQuarie and Simon, Viva, NewDelhi, (2001).
2. Chemical Kinetics-K. J. Laidler, McGraw Hill.Inc. New York (1988).
3. Principles of Chemical Kinetics– House J. E. Wm C Brown Publisher, Boston, (1997).
4. Physical Chemistry-P. Atkins and J. D. Paula, 9<sup>th</sup> Edn. Oxford University Press (2010).
5. Modern Electrochemistry Vol-1 and 2 J. O'. M Bockris and A. K. N.Raddy, Plenum New York (1978).



6. Text book of physical chemistry Samuel Glastone, 2<sup>nd</sup> edition, Mac Millan India Ltd (1991).
7. Principles and applications of Electrochemistry-D. R. Crow 3<sup>rd</sup> edition Chapman hall London (1988).
8. A Textbook of physical Chemistry Vol-2, 3 and 5- K. L. Kapoor 5<sup>th</sup> edition Mcgraw Higher Ed (2015)

#### SUGGESTED REFERENCE BOOKS

1. Kinetics and Mechanism of Chemical Transformations-J. Rajaraman and J. Kuriakose, Mc Millan. (1986).
2. Biological Chemistry by James P Allen, Wiley-Blackwell, 2008.
3. Introduction to Biophysical Chemistry, R. Bruce Martin, McGraw-Hill, NY, 1964.
4. Physical Chemistry with applications to biological systems, Ramond Chnag, Mc Millan publishing Co.inc, New York 1977.
5. Molecular Modelling: Principle and Application, 2<sup>nd</sup> Ed. by Andrew R. Leach, Addison-Wesley Longman Ltd. 2009. K
6. Kinetics and Mechanism—A. A. Frost and R.G.Pearson, John-Wiley, New York, (1961).
7. S.H.Maranand C.F.Pruton, 4<sup>th</sup> Edn. Oxford & IBH publishing Co. Pvt. Ltd. New Delhi (1965).

| Course Title: Inorganic Chemistry Lab |                                                     |                 |              |
|---------------------------------------|-----------------------------------------------------|-----------------|--------------|
| Course Code                           | CHE81DC01104                                        | Credits         | 4            |
| L + T + P                             | 0 + 0 + 8                                           | Course Duration | One Semester |
| Semester                              | Odd                                                 | Contact Hours   | 120 Hours    |
| Methods of Content Interaction        | Lecture, Reagents Preparation and Practical Classes |                 |              |

#### OBJECTIVE:

- To make students proficient in qualitative analysis of acidic and basic radicals including rare ones such as W, Zr, U, Ce, Mo etc
- To impart effective training in synthesis of inorganic complexes and its characterization using various instrumental techniques such as UV-Vis-NIR absorption and luminescence spectroscopy, FTIR spectroscopy, TG/DTA analysis etc.
- To equip the students with necessary skills in quantitative analysis

#### Learning Outcomes

After completion of the course the learners will be able to:

- Find the cations and anions present in a given sample
- Synthesize inorganic complexes of various types and characterize it using instrumental techniques
- Determine, quantitatively, the amount of metals present in an ore, alloy or solution

\*Few experiments will be set from each section depending on the availability of chemicals.

**Lab-I: Qualitative Analysis**

Semimicro qualitative analysis of mixtures containing one anion, one common cation and one less familiar element: W, Mo, Ce, Th, Zr, V, U and Li.

**Lab-II: Synthesis and characterization of inorganic complexes**

Preparation and quantitative analysis of inorganic complexes:

1. *Cis*- and *trans*-potassiumdioxalatodiaquachromium(III) complex [analysis of oxalate and chromium]
2. Hexamminecobalt(III)chloride [analysis of cobalt]

**Lab-III: Quantitative analysis of metals in alloys, ores and solution Gravimetric analysis**

1. Gravimetric determination of Fe in iron ore as Fe<sub>2</sub>O<sub>3</sub>.
2. Gravimetric determination of Ni in Cu and Ni solution.
3. Gravimetric determination of Fe in Fe and Cr solution.

**Volumetric analysis**

1. Volumetric estimation of Ca and Mg in Dolomite solution.
2. Volumetric estimation of Cu in Cu and Ni (German silver).
3. Volumetric estimation of Fe in Cu and Fe solution.

**SECOND SEMESTER (EVEN SEMESTER)**

| Course Title: Photochemical and magnetic properties of complexes |                                                                          |                 |                       |
|------------------------------------------------------------------|--------------------------------------------------------------------------|-----------------|-----------------------|
| Course Code                                                      | CHE82DC01204                                                             | Credits         | 4                     |
| L + T + P                                                        | 3 + 1 + 0                                                                | Course Duration | One Semester          |
| Semester                                                         | Even                                                                     | Contact Hours   | 45 (L) + 15 (T) Hours |
| Methods of Content Interaction                                   | Lecture, Tutorials, Group discussion; self-study, seminar, presentations |                 |                       |

**Course Objectives**

- To make students understand the structure and properties of inorganic chains, rings and sheets
- To equip the students with necessary skills in electronic spectroscopy of metal complexes
- To acquaint the students with the photochemical reactions of coordination compounds
- To introduce the core concepts of magnetochemistry for analysing properties of complexes

**Learning Outcomes:** After completion of the course the learners will be able to:

- Analyse the optical/electronic spectra of coordination compounds
- Make use of the photochemical behaviour of complexes in designing solar cells
- Design and perform photochemical reactions of metal complexes
- Analyse the magnetic properties of complexes
- Explain the various phenomena taking place in the nucleus

- Understand the working of nuclear reactors
- Utilize various nuclear techniques for analytical and biomedical applications

### UNIT-I

**Chemistry of main group elements-** Structure and bonding in boranes, carboranes, metallocarboranes, Wade's rules, Wades-Mingos and Lauher rules, borazines, P, N and S compounds.

**Silicates-** Classification, structures, isomorphous replacement, pyroxenes, layered and vitreous silicates, zeolites and molecular sieves.

### UNIT-II

**Electronic spectra of coordination compounds-** Spectroscopic ground states, selection rules, term symbols for dn ions, Racah parameters, Orgel, Correlation and Tanabe-Sugano diagrams, spectra of 3d metal-aqua complexes of trivalent V, Cr, divalent Mn, Co and Ni,  $\text{CoCl}_4$ , calculation of  $Dq$ ,  $B$  and  $\beta$  parameters, CT spectra. Spectral properties of Lanthanide and Actinide metal complexes.

### UNIT-III

**Photochemical reactions of transition metals complexes:** Basic photochemical processes, Kasha's rule, quantum yield, Jablonskii diagrams, photo substitution reactions, photo-redox reactions, ligand photoreactions, photo reactions and solar energy conversion.

### UNIT-IV

**Magnetic properties of coordination compounds-** Types of magnetic behaviour, magnetic susceptibility and its determination-Gouy, Faraday, VSM method. Diamagnetic correction, orbital contribution, spin-orbital coupling, ferro- and antiferromagnetic coupling, spin-crossover. Magnetic properties of Lanthanide and Actinide metal complexes.

### SUGGESTED TEXT BOOKS

1. Basic Inorganic Chemistry- F. A. Cotton, G. Wilkinson and P. L. Gaus; John Wiley and sons. Inc, 2007.
2. Chemistry of elements-N. N. Greenwood and A. E. Earnshaw, Butterworth Heinemann (1997).
3. Inorganic Chemistry IV edition; J. E. Huheey, E. A. Keiter and R. L. Keiter, Addison; Wesley, 2008.
4. Inorganic Chemistry, III edition, D. F. Shriver, P. W. Atkins and C. H. Langford, ELBS; Oxford University Press, 1999.
5. Inorganic Electronic spectroscopy, A. B. P. Lever, Elsevier. (1968).
6. Magnetochemistry, R.L. Carlin, Springer Verlag, 1986.
7. Electronic Absorption Spectroscopy and related Techniques, D. N. Sathyanarayana, University Press (2001).
8. Inorganic Chemistry a Unified Approach by W. W. Porterfield, Elsevier 2005 2<sup>nd</sup> edition.
9. Textbook of inorganic chemistry by G. S. Sodhi, Viva books Pvt. Ltd (2011).

| <b>Course Title: Reaction Mechanism (II), Pericyclic and Photochemical Reactions</b> |                                                                          |                        |                          |
|--------------------------------------------------------------------------------------|--------------------------------------------------------------------------|------------------------|--------------------------|
| <b>Course Code</b>                                                                   | <b>CHE82DC02204</b>                                                      | <b>Credits</b>         | 4                        |
| <b>L + T + P</b>                                                                     | 3 + 1 + 0                                                                | <b>Course Duration</b> | One Semester             |
| <b>Semester</b>                                                                      | Even                                                                     | <b>Contact Hours</b>   | 45 (L) + 15 (T)<br>Hours |
| <b>Methods of Content Interaction</b>                                                | Lecture, Tutorials, Group discussion; self-study, seminar, presentations |                        |                          |

**OBJECTIVE:** To develop the concepts in depth about reaction mechanisms related to substitution, addition, elimination, and rearrangement reaction. To give an idea about pericyclic reactions and photochemical processes/reactions and their application in organic synthesis.

**Learning Outcomes:** After completion of the course the learners will be able to:

- Here students will know the depth of knowledge of reactive intermediates in organic reactions, and different kinds of reactions such as substitution, elimination, rearrangement reactions, and their application in organic synthesis.
- Students will be able to understand the unique photochemical process and its role in organic synthesis.
- Students will be able to get knowledge of pericyclic reactions, their mechanism, and use in the synthesis of different kinds of organic molecules.

### UNIT-I

**Reactive Intermediates and their chemistry:** General introduction of reactive intermediates. Generation, structure, stability and reactivity of common reactive intermediates. Detailed reactions and application of carbenes, free radicals, nitrenes and benzynes.

### UNIT-II

#### Substitution Reactions

**Aliphatic and aromatic Electrophilic Substitution Reactions:** The arenium ion mechanism. Orientation and reactivity. Energy profile diagrams. The *ortho* / *para* ratio, *ipso* attack, orientation in other ring systems. Quantitative treatment of reactivity in substrates and electrophiles. Effect of leaving group.

Substitution at allylic carbon (allylic rearrangement), at a trigonal carbon (hydrolysis of esters and amides), and substitution at a vinylic carbon. Neighboring group participation and  $S_Ni$  reactions, non-classical carbonium ion.

**Aliphatic and Aromatic Nucleophilic substitution reactions:** The  $S_NAr$ ,  $S_N1$ , benzyne and  $SR_N1$  mechanisms. Reactivity: effect of substrate structure, leaving group and attacking nucleophile. Goldberg reaction, Bucherer reaction, Schiemann reaction, von Richter reaction, Sommelet-Hauser and Smiles rearrangements.

$S_E2$ ,  $S_E1$  and  $S_Ei$  mechanisms. Hydrogen exchange, migration of double bonds,  $\alpha$ -halogenation of aldehydes, ketones and acids. diazo transfer reaction,

## Rearrangements:

General Mechanistic considerations-nature of migration, migratory aptitude, memory effects. Wagner-Meerwein, Pinacol-Pinacolone, Fries, Wolff, Beckmann, Hofmann, Curtius, Lossen and Schmidt rearrangements. Benzil-benzilic acid rearrangement, Arndt-Eistert reaction, Tiffeneau-Demjanov reaction, Fritsch-Buttenberg-Wiechell rearrangement. Stevens, Wittig and Favorskii rearrangements, Dienone-phenol, Baker-Venkatraman rearrangement. Baeyer-Villiger oxidation. Neber rearrangement. Benzidine rearrangement.

## UNIT-III

**Photochemistry:** Physical and Chemical processes, Jablonski diagram. Photosensitization, quantum efficiency, quantum and chemical yields, solvent effects, Stern-Volmer plot, delayed fluorescence etc.

### Photochemistry of functional groups:

(A) **Olefins:** Cis-trans isomerism, [2+2]-cycloaddition, rearrangements. Reaction of conjugated olefins; di-methane rearrangements (including oxo- and aza-di-methane rearrangements).

(B) **Ketones:** Excited state of C=O. Norrish type-I and type-II cleavages. Paterno-Buchi reaction.  $\alpha$ -unsaturated ketones. [2+2] addition. Rearrangement of cyclohexadienones (application in the synthesis of some important natural products).

(C) **Aromatic compounds:** Photorearrangement of benzene and its derivatives, cycloaddition of benzene.

(D) **Photochemical oxidations and reductions:** Cycloaddition of singlet molecular oxygen {[2+2], [4+2]-additions}. Oxidative coupling of aromatic compounds, photoreduction by hydrogen abstraction

## UNIT-IV

**Pericyclic reactions** Molecular orbital symmetry, Woodward-Hoffmann correlation diagrams. FMO and PMO, Conservation of orbital symmetry approaches. Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl system. Electrocyclic reactions: conrotatory and disrotatory motions,  $4n$ ,  $4n+2$  and allyl systems.

**Cycloadditions:** antarafacial and suprafacial additions,  $[\pi m s + \pi n a]$  and  $[\pi m s + \pi n s]$ -cycloadditions.  $[\omega 2 a + \pi 2 s]$  and  $[\pi 4 s + \omega 2 s]$ -cheletropic reactions. Regio, enantio and Endoselectivities in Diels-Alder reactions. Hetero Diels-Alder reaction.

**Sigmatropic rearrangements:** suprafacial and antarafacial shifts of H, sigma-tropic shifts involving carbon moieties.  $[i, j]$ -Sigmatropic rearrangements (including Walk, Claisen, Cope, oxy and aza-Cope rearrangements), Ene reaction.

## SUGGESTED TEXT BOOKS

1. Advanced Organic Chemistry—Reactions, Mechanism and Structure, Jerry March, John Wiley (2008).
2. Advanced Organic Chemistry, F.A. Carey and R.J. Sundberg, Volume A and B, 2008.
3. A Guide Book to Mechanism of Organic Chemistry, Peter Sykes, Longman (2000).
4. Organic Chemistry, R. T. Morrison and R. N. Boyd, Prentice-Hall (1998).

- Principles of Organic Synthesis, R.C. Norman and J. M. Coxon, Blackie Academic and Professional, 2012.
- Stereochemistry of Organic Compounds, D. Nasipuri, New-Age International (1999).
- Molecular Reactions and Photo chemistry by Depuy and Chapman.

#### SUGGESTED REFERENCE BOOKS

- Frontier Orbitals and Organic Chemical Reactions, I. Fleming, Wiley, London, 1976.
- Pericyclic Reactions- A text Book, S. Sankararaman, Wiley VCH, 200.
- Organic Photochemistry, J. M. Cozen and B. Halton, Cambridge University Press (1<sup>st</sup> Edition) 1974.
- Organic Chemistry, Volumes I and II, I L Finar, Longman.(1999).
- Reagents in Organic synthesis by B .P. Mundy and others.
- Named Reactions by Jie Jack Li.
- Stereochemistry of Carbon Compounds, E.L. Eliel, S. H. Wilen and L. N.Mander, John Wiley (1994).

| Course Title: Quantum Chemistry |                                                                          |                 |                       |
|---------------------------------|--------------------------------------------------------------------------|-----------------|-----------------------|
| Course Code                     | CHE82DC03204                                                             | Credits         | 4                     |
| L + T + P                       | 3 + 1 + 0                                                                | Course Duration | One Semester          |
| Semester                        | Even                                                                     | Contact Hours   | 45 (L) + 15 (T) Hours |
| Methods of Content Interaction  | Lecture, Tutorials, Group discussion; self-study, seminar, presentations |                 |                       |

#### Course Objectives

- To equip the students with the skills in quantum mechanics
- To lay the foundations of quantum mechanics by giving the mathematical background and concept of operators.
- To make the students understand the Quantum mechanical treatment of translational, rotational and vibrational motion through models such as particle in a box(1-D, 2D, 3D), rigid rotor, harmonic oscillator
- To develop a comprehensive understanding of a single electronic and multielectronic systems including spectroscopic transitions.

**Learning Outcomes:** After completion of the course the learners will be able to:

- Formulate and solve quantum mechanical equations for a given system
- Analyse a given situation from quantum mechanical viewpoint and write appropriate Schrodinger equation

#### UNIT-I

**Mathematical Concepts:** Logarithmic relations, curve sketching, linear graphs and calculation of slopes, differentiation of functions like  $f(x)$ ,  $e^x$ ,  $x^n$ ,  $\sin x$ ,  $\log x$ ; maxima and

minima, partial differentiation and reciprocity relations. Integration of some useful / relevant functions, permutations and combinations, factorials and probability.

**Concepts of Operators:** Laplacian, Hamiltonian, Linear and Hermitian operators. Angular momentum operators and their properties. Commutation of operators. Normalization, orthogonality and orthonormality of wave functions. Average (expectation) values

## UNIT -II

**Quantum Mechanics-I:** Introduction to quantum mechanics. Schrödinger wave equation. Time-independent and time-dependent Schrödinger wave equations and the relation between their solutions. Eigen functions and Eigen values. Physical Interpretation of wave function.

Postulates of quantum mechanics. Solutions of Schrödinger wave equation for a free particle, particle in a three-dimensional box. Quantum mechanical degeneracy, tunnelling (no derivation). Application of Schrödinger equation to harmonic oscillator, rigid rotator. Eigen functions and eigen values of angular momentum. Ladder operator method for angular momentum.

## UNIT -III

**Quantum Mechanics-II:** Schrödinger equation to hydrogen atom in spherical polar coordinates. Solution of  $\Phi$ ,  $\Theta$  equation and statements of solution of  $R$  equation. Total wave functions of hydrogen atom. Quantum numbers and their characteristics. List of wave functions for few initial states of hydrogen like atoms. Diagrams of radial and angular wave functions. Radial and angular probability functions and their significance. Electron spin (Stern-Gerlach experiment), spin-orbital, anti-symmetry and Pauli-exclusion principle, Slater determinants.

## UNIT-IV

**Methods of Approximation:** Need for approximate methods. Perturbation method. Rayleigh Schrödinger perturbation theory for time-independent non-degenerate system. Application to electron in a box under the influence of an electric field. Application to He atom. Variation theory-statement and proof. Application of variation method to particle in a one-dimensional box and He atom.

**Spectroscopic Transitions:** Time dependent Schrodinger equation, origin of selection rules, Coupling of angular momenta. Russell-Saunders and JJ-coupling, Term symbols. Spin-orbital interaction and explanation of term multiplicities, Zeeman effect.

## SUGGESTED TEXT BOOKS

1. Quantum Chemistry: Donald A. McQuarrie University Science Books, 2<sup>nd</sup> edition (2008).
2. Introduction to Quantum Chemistry, A. K. Chandra, Tata Mc GrawHill, (1988).
3. Quantum Chemistry, Ira. N. Levine, Prentice Hall, New Jersey, (1991).
4. Quantum Chemistry, R.K. Prasad, New Age International, 2<sup>nd</sup> edition, (2000).
5. Quanta, Matter, and Change: A Molecular Approach to Physical Chemistry, Peter Atkins, Julio de Paula, Ronald Friedman, Oxford Univ. Press (2009)
6. Quantum Chemistry, R.K. Prasad, New Age International, 2<sup>nd</sup> edition, (2000).

## SUGGESTED REFERENCE BOOKS

1. Molecular Quantum Mechanics, P. W. Atkins and R. Friedman, Oxford Univ. Press, 5<sup>th</sup> edition (2011)
2. Quantum Chemistry, J. P. Lowe, K.A. Peterson, Elsevier, 3<sup>rd</sup> Edition (2006).
3. Atoms, Molecules and Photons, W. Demtröder, 2<sup>nd</sup> edition, Springer (2010).

| Course Title: Research Methodology |                                                   |                 |                       |
|------------------------------------|---------------------------------------------------|-----------------|-----------------------|
| Course Code                        | CHE82DC04004                                      | Credits         | 4                     |
| L + T + P                          | 3 + 1 + 0                                         | Course Duration | One Semester          |
| Semester                           | Even                                              | Contact Hours   | 45 (L) + 15 (T) Hours |
| Methods of Content Interaction     | Lecture, Reagents Preparation and Practical Class |                 |                       |

**Course objectives:** This course is designed to provide an overview on fundamentals of doing research including scientific terminology, literature, methods, analysis, and interpretation of data, preparation of research report and presentation, future aspects of research as a career, importance, and applications of scientific research to the society.

It will help the students to develop core research skills relevant to a wide spectrum of chemical research including written and oral communication, skills in making scientific observations, and recording and analysing data by participating in discussions or through presentations or group research project associated with a discipline of interest to them. Assignments and tutorials would be included to enhance the course deliver and outcome.

## UNIT I

### Principles of Research

**Foundation of Research:** Objectives of scientific research, research & theory-conceptual and theoretical model, importance of research methodology in scientific research, types and methods of research, evaluation of research/study.

**Research problem:** meaning of research problems, sources of research problems, criteria/ characteristics of a good research problem, errors in selecting a research problem.

**Hypothesis:** Meaning, types of hypothesis.

Design and execution of experiments, collection and interpretation of experimental data, arriving at conclusions.

Errors in chemical analysis, classification of errors, determination of accuracy of methods, improving accuracy of analysis, significant figures, mean, standard deviation.

## UNIT II

### Literature Survey and Software

**Print:** Sources of information need for reviewing literature, primary-secondary and tertiary sources, journals, journal abbreviations, abstracts, current titles, reviews, monographs, dictionaries, text books, current contents, and patents. Introduction to chemical abstracts and beilstein, subject index, substance index, author index, formula index and other indices with examples.



**Digital:** Web resources, E-journals, journal access, TOC alerts. Hot articles: Citation index, UGC infonet, E-books, Impact Factors

**Search engines:** Google scholar, chemical industry, Wiki-databases, chemSpider, ScienceDirect, SciFinder, Scopus etc.

**Software Application in Chemistry:** Use of ChemDraw and Microsoft chemistry add-in software, use of reference tab in MS word, Mendeley, Zotero, EndNote etc, creating table of content, adding footnote and caption.

Use of spreadsheet (Excel) for simple calculations, plotting graphs using a spreadsheet (radial distribution curves for hydrogenic orbitals, gas kinetic theory, pressure-volume curves of vander Waals gas, graphical solution of equations), solving equations numerically (e.g. pH of a weak acid ignoring/not ignoring the ionization of water, volume of a vander Waals gas, equilibrium constant expressions).

**Use of Origin software.**

### UNIT III:

#### Concepts of Chemical Safety

Chemical safety and ethical handling of chemicals, safe working procedure and protective environment, emergency procedure and first aid, laboratory ventilation, safe storage and use of hazardous chemicals, procedure for working with substances that pose hazards, flammable or explosive hazards, procedures for working with gases at pressures above or below atmosphere, safe storage and disposal of waste chemicals, recovery, recycling, and reuse of laboratory chemicals.

### UNIT IV

#### Research Literature and Seminar

The art of scientific communication, presentation in seminars and conferences. This part of the course will be conducted as a Journal Club. Students will be expected to read and summarize a research paper from the recent literature. The student will familiarize himself/herself with the background necessary to understand the research paper, and will be expected to critically analyze the work and to answer questions from other students and from the faculty moderator(s).

### SUGGESTED REFERENCE BOOKS

1. Practical Skills in Chemistry, J. R. Dean, A. M. Jones, D. Holmes, R. Reed, J. Weyers and A Jones, Pearson Education Ltd., Prentice Hall, (2002).
2. Research Methodology. Methods and Techniques: C. R. Kothari.
3. Paul D Leedy, Jeanne E Ormrod and Jeanne Ellis Ormrod, Practical Research: Planning and Design, Prentice Hall, 2004.
4. Robert V Smith, Graduate Research: A Guide for Students in the Sciences, University of Washington Press, 1998.
5. Biggs Pete, Computers in Chemistry, Oxford University Press, 2000.
6. Cropper William H, Mathematical Computer Programs for Physical Chemistry, Springer.
7. Chemical Safety Manual, IIT Bombay.  
<http://www.iitb.ac.in/safety/sites/default/files/chemical%20safety%20manual.pdf>.

8. Chemical Safety Manual, ACS.  
<https://www.acs.org/content/dam/acsorg/about/governance/committees/chemicalsafety/publications/chemical-safety-manual-teachers.pdf>.
9. Fundamentals of Analytical Chemistry, 2013, D. Skoog.
10. Instrumental Methods of Analysis, Willard

| <b>Course Title: Physical Chemistry Lab</b> |                                                   |                        |              |
|---------------------------------------------|---------------------------------------------------|------------------------|--------------|
| <b>Course Code</b>                          | <b>CHE82DC03104</b>                               | <b>Credits</b>         | 4            |
| <b>L + T + P</b>                            | 0 + 0 + 8                                         | <b>Course Duration</b> | One Semester |
| <b>Semester</b>                             | Even                                              | <b>Contact Hours</b>   | 120 Hours    |
| <b>Methods of Content Interaction</b>       | Lecture, Reagents Preparation and Practical Class |                        |              |

### Course Objectives

To equip the students with necessary laboratory skills for performing experiments of chemical kinetics and catalysis

- To acquaint students with basics of computational chemistry and molecular modelling
- To make the students proficient in drawing stereochemical structure of a molecules using software tools such as ChemDraw, ChemOffice
- To impart training to the students in various instrumental techniques such as conductometry, potentiometry, UV-Vis spectrophotometry, FTIR spectroscopy and cyclic voltametry.
- To make students learn how to perform qualitative and quantitative analysis using such equipment.

**Learning Outcomes:** After completion of the course the learners will be able to:

- Determine the activation energy, rate constant and equilibrium constant of different reactions using various instrumental techniques.

### Lab-I

1. Comparison of acid strength (HCl and H<sub>2</sub>SO<sub>4</sub>) by studying acid-catalysed hydrolysis of methyl acetate at lab temperature.
2. Determination of rate constant and energy of activation for the base hydrolysis of ethylacetate Verification of Beer's Law for Cu<sup>2+</sup> and Fe<sup>2+</sup> ions
3. Estimation of Fe<sup>2+</sup> ions concentration in the given solution by titration of FAS versus KMnO<sub>4</sub> through colorimetric method.
4. Estimation of Fe<sup>2+</sup> ions concentration using EDTA through colorimetric method.
5. Phase diagram of two component systems and determination of E<sub>C</sub>, E<sub>T</sub> and the determination of the composition of given unknown.
6. Determination of partial molar volume of solute-H<sub>2</sub>O system by apparent molar volume method.
7. Determination of the viscosity of a mixture by apparent molar volume method.

8. Verification of Freundlich and Langmuir isotherms for adsorption of oxalic / acetic acid on activated charcoal.

### **Lab-II**

1. Study the hydrolysis of methyl acetate at two different concentrations of HCl and report the relative strength.
2. Determination of dissociation constant of a given indicator by colorimetric method.
3. Study of kinetics of auto catalytic reaction between  $\text{KMnO}_4$  versus oxalic acid.
4. Determination of degree of hydrolysis of aniline hydrochloride at room temperature and calculation of dissociation constant of the base by pH-metry
5. Study of variation of viscosity of a liquid with temperature, determine the constant A and B.
6. Analysis of a binary mixture of two miscible liquids and to determine the composition of the given unknown mixture.
7. Evaluation of Arrhenius parameter for the reaction between  $\text{K}_2\text{S}_2\text{O}_8$  versus KI (first order)

### **Lab -III**

#### **Conductometry**

1. Conductometric titration of strong acid with strong base
2. Conductometric titration of weak acid with strong base
3. Conductometric titration of oxalic acid with strong base
4. Conductometric titration of acid mixture with strong base
5. Conductometric titration of  $\text{AgNO}_3$  with KCl
6. Conductometric titration of  $\text{BaCl}_2$  with  $\text{Na}_2\text{SO}_4$
7. Determination of Molar and Equivalent conductivity of a given strong electrolyte (and weak electrolyte) as a function of concentration

#### **Potentiometry**

1. Determination of strength of HCl,  $\text{CH}_3\text{COOH}$  and oxalic acid versus NaOH by pH-metry
2. To determine the acidic and basic dissociation constant of an amino acid and determination of isoelectric point by pH-metry.
3. Determination of dissociation constant of  $\text{H}_3\text{PO}_4$  using potentiometric / pH-metric method.
4. Determination of strength of  $\text{Fe}^{2+}$  solution by performing potentiometric titration with  $\text{K}_2\text{Cr}_2\text{O}_7$  or  $\text{KMnO}_4$
5. pH-metric titration of mixture of weak and strong acid against NaOH
6. Determination of stability constant of copper-ethylenediamine complex by potentiometry
7. Determination of  $\text{pK}_a$  of amino acids by potentiometric titration

## Lab -IV

### Additional experiments based on cyclic voltametry and electrogravimetry

1. Estimation of copper by electrogravimetric method
2. Polarographic analysis, identification and estimation of metal ions ( $\text{Pb}^{2+}$ ,  $\text{Cd}^{2+}$ ,  $\text{Zn}^{2+}$ )
3. Cyclic voltammetry of a standard redox couple (ferricyanide-ferrocyanide couple)

### SUGGESTED BOOKS

1. Practicals in Physical Chemistry, P S Sindhu, Macmillan, 2005
2. Practical Physical Chemistry, Alexander Findlay, CHIZINE PUBN, 2018
3. Experimental Physical Chemistry: A Laboratory Textbook, Arthur Halpern, George McBane, I. W. H. Freeman, 2006
4. Experiments in Physical Chemistry: Second Revised and Enlarged Edition, J. M. Wilson, R. J. Newcombe, A. R. Denaro, Elsevier, 2016
5. Experimental Physical Chemistry - Scholar's Choice Edition, Daniels Farrington, Scholar's Choice, 2015
6. Quantitative Chemical Analysis, 9<sup>th</sup> edition, Daniel C. Harris, W. H. Freeman, 2015
7. Vogels Textbook of Quantitative Chemical Analysis, Mendham, Pearson Education India, 2006

### **THIRD SEMESTER (Odd SEMESTER)**

| Course Title: Organic Chemistry Lab |                                           |                 |              |
|-------------------------------------|-------------------------------------------|-----------------|--------------|
| Course Code                         | CHE91DC02104                              | Credits         | 4            |
| L + T + P                           | 0 + 0 + 8                                 | Course Duration | One Semester |
| Semester                            | Odd                                       | Contact Hours   | 120 Hours    |
| Methods of Content Interaction      | Lecture, Reagents Preparation, Practicals |                 |              |

**OBJECTIVE:** To develop skills of synthesis, purifications and characterisation of organic compounds.

\*Few experiments from each section will be set to perform the experiments depending on the availability of chemicals.

### Organic Chemistry Practical-I: Preparation (One stage)

1. Cannizarro reaction: Benzaldehyde.
2. Fries rearrangement: Phenyl acetate.
3. Friedel-Crafts reaction: Benzene and Acetylchloride.
4. Sandmeyer reaction: 4-Chlorotoluene from 4-toluidine.
5. Oxidation of Cyclohexanol.
6. Preparation of S-Benzylisothiuroniumchloride.

7. Synthesis of *p*-iodonitrobenzene
8. Synthesis of *N*-Phenyl-2,4-dinitroaniline.
9. Synthesis of 2,4,6-tribromoaniline.
10. Synthesis of 2,4-dichlorophenoxyacetic acid.

Purification of above compounds (products) by –crystallization, fractional crystallization, distillation, fractional distillation, vacuum distillation and column chromatography. Use of TLC for identification of Organic compounds.

### **Organic Chemistry Practical-II**

Small scale organic synthesis using some of the following reactions:

- i. Acetylation reaction
- ii. Oxidations and reductions
- iii. Nucleophilic aromatic/aliphatic substitution
- iv. Bromination and bromine addition
- v. Condensations
- vi. Diazotisation reactions

### **Organic Chemistry Practical-III: Simple Instrumental techniques in Organic Chemistry**

1. Determination of specific rotation of given compounds and of racemic mixture
2. Determination of  $pK_a$  of amino acids by potentiometric titration
3. Estimation of a common drug (paracetamol) by UV spectroscopy
4. Estimation of Keto-enol tautomerism by IR
5. Separation of amino acids by thin layer chromatography
6. Separation of proteins by gel electrophoresis
7. Estimation of protein in food samples
8. Estimation of Vitamin A in food samples
9. Determination of concentration of chiral compounds

### **Organic Chemistry Practical-IV:**

(A) Preparations of various organic compounds employing different reactions such as

1. Diels-Alder reaction between furan and maleic acid,
2. Thiamine hydrochloride catalyzed benzoin condensation,
3. Pechmann condensation for coumarin synthesis,
4. Electrophilic aromatic substitution reaction,
5. Radical Coupling reaction,
6. Three component coupling reaction etc

Products should be characterized using UV, IR and NMR technique with a view to give the student sufficient training in synthetic organic chemistry.

## SUGGESTED TEXT BOOKS

1. A Text Book of Quantitative Inorganic Analysis: A. I. Vogel, 1989.
2. Vogel A. I. *Practical Organic Chemistry*, Longman Group Ltd.
3. Bansal R. K. *Laboratory Manual of Organic Chemistry*, Wiley-Eastern.
4. Ahluwalia V. K. and Aggarwal R. *Comprehensive practical organic chemistry*, University press.
5. Nad A. K.; Mahapatra B. and Ghoshal A. *An advanced course in practical chemistry*, New Central Book Agency (P) Ltd.
6. Wilson, John H. Block, Ole Givold, John Marlowe Beale, 2004.

| Course Title: Molecular Spectroscopy |                                                                          |                 |                          |
|--------------------------------------|--------------------------------------------------------------------------|-----------------|--------------------------|
| Course Code                          | CHE91DC03304                                                             | Credits         | 4                        |
| L + T + P                            | 3 + 1 + 0                                                                | Course Duration | One Semester             |
| Semester                             | Odd                                                                      | Contact Hours   | 45 (L) + 15 (T)<br>Hours |
| Methods of Content Interaction       | Lecture, Tutorials, Group discussion; self-study, seminar, presentations |                 |                          |

### Course Objectives

- To equip the students with necessary knowledge and skills in spectroscopy, namely, rotational, vibrational and electronic spectroscopy
- Learning Outcomes:** After completion of the course the learners will be able to:
- Analyse spectroscopic data for identification of compound and use it for understanding intermolecular interactions.

## UNIT I

**Introduction to spectroscopy:** regions of electromagnetic spectrum, understanding photons as a boson, oscillating dipole in a molecule, the light-matter interaction, conservation of angular momentum, signal to noise ratio, resolving power, width and intensity of spectroscopic transitions, Beer-Lambert law

**Rotational Spectroscopy:** Rotations of molecules, rigid diatomic molecule-rotational energy expression, energy level diagram, rotational wave function and their symmetry, selection rules, expression for the energies of spectral lines, computation of intensities, effect of isotopic substitution, centrifugal distortion and the spectrum of a non-rigid rotor. Rotational spectra of polyatomic molecules-linear, symmetric top and asymmetric top molecules. Nuclear effects in rotational spectroscopy.

## UNIT-II

**Infrared Spectroscopy-I:** Vibrations of molecules, harmonic and anharmonic oscillators-vibrational energy expression, energy level diagram, vibrational wavefunctions and their symmetry, selection rules, expression for the energies of spectral lines, computation of intensities, hot bands, effect of isotopic substitution. Diatomic vibrating rotor, Born-Oppenheimer approximation, vibrational-rotational spectra of diatomic molecules, P, Q and R branches, breakdown of the Born-Oppenheimer approximation.

**Infrared Spectroscopy-II:** Vibrations of polyatomic molecules: Normal coordinates translations, vibrations and rotations, vibrational energy levels and wave functions, fundamentals, overtones and combinations. Vibration- rotation spectra of polyatomic molecules- parallel and perpendicular vibrations of linear and symmetric top molecules Techniques and instrumentation.

**FTIR spectrometer:** construction of the instrument, dispersive and non-dispersive spectrometers, change dipole moments during molecular vibrations, Interferogram and its Fourier Transformation, Far-IR, Mid-IR, Near IR spectral regions, optical windows: KBr, CsI pellet technique, Paraffin mulls, ZnSe, CaF<sub>2</sub> windows; Total internal reflectance based devices.

### UNIT-III

**Electronic Spectroscopy:** Born-Oppenheimer approximation, vibrational coarse structure, intensities by Franck- Condon principle, Dissociation energy, rotational fine structure, Fortrat diagram, pre-dissociation, Electronic structure of diatomic molecules-basic results of MO theory, classification of states by electronic angular momentum- and molecular orbitals, selection rules, spectrum of singlet and triplet molecular hydrogen, Electronic spectra of polyatomic molecules-localized MOs, spectrum of HCHO, change of shape on excitation, Decay of excited states-radioative (fluorescence and phosphorescence) and non-radioative decay, internal conversion.

**UV-Vis Absorption and Fluorescence Spectrophotometer:** construction of the instrument, measuring a spectrum, Beer-Lambert law, deviations from Beer's law, Relating UV-Vis spectra and colour, spectroscopic monitoring of titrations and kinetics. Fluorescence quantum yield measurement.

### UNIT-IV

**Raman Spectroscopy:** Rayleigh and Raman Scattering, classical and quantum mechanical view point; Vibrational Raman spectroscopy, Stokes and Anti-Stokes lines, mechanistic aspects, polarizability, electric field and induced dipole, Raman active/inactive vibrations / rotations in molecules, polarizability ellipsoid, mutual exclusion principle, polarized Raman lines during vibration, Combined Raman and infrared spectra for structural determination; Rotational Raman spectroscopy, selection rules, spectra of symmetric top and spherical top molecules. Resonance Raman Spectroscopy

**Raman Spectrometer:** instrumentation, measuring a spectrum, lasers and their use in Raman spectroscopy.

### SUGGESTED BOOKS

1. Introduction to Molecular Spectroscopy, C. N. Banwell, TMH Edition (1994).
2. Introduction to Molecular Spectroscopy, G.M. Barrow, McGraw Hill (Int. Students Edition) (1988).
3. Molecular Spectroscopy, J. D. Graybeal, McGraw Hill (Int. Students Edition) (1990).
4. Spectroscopy, Vols. 1-3, B. P. Straughan and W. Walker, Chapman Hall (1976).

| <b>Course Title: Inorganic Materials and Their Applications</b> |                                                                          |                        |                       |
|-----------------------------------------------------------------|--------------------------------------------------------------------------|------------------------|-----------------------|
| <b>Course Code</b>                                              | <b>CHE91DC01304</b>                                                      | <b>Credits</b>         | 4                     |
| <b>L + T + P</b>                                                | 3 + 1 + 0                                                                | <b>Course Duration</b> | One Semester          |
| <b>Semester</b>                                                 | Odd                                                                      | <b>Contact Hours</b>   | 45 (L) + 15 (T) Hours |
| <b>Methods of Content Interaction</b>                           | Lecture, Tutorials, Group discussion; self-study, seminar, presentations |                        |                       |

### Course Objectives

- To enhance the understanding of the electronic structure of solids
- To acquaint the students with the advanced level concepts in magnetochemistry such as magnetic anisotropy and single molecule magnets
- To familiarize the students with the concepts of piezoelectricity, ferroelectricity, dielectrics and superconductivity
- To impart the knowledge and skills in electrochemical aspects of inorganic systems

**Learning Outcomes:** After completion of the course the learners will be able to:

- Distinguish between piezoelectric and ferroelectric effects in inorganic systems
- Understand and apply concepts of piezoelectricity, ferroelectricity in daily life
- Determine the magnetic anisotropy and susceptibility in inorganic systems
- Apply the advanced concepts in designing single molecule magnets
- Apply the concepts of defects-engineering to obtain enhanced features of inorganic systems
- Explain the electrochemical processes occurring in biological systems
- Apply the concepts for protection from corrosion

## UNIT-I

**Electronic structure of solids:** Bonding in solids: Ionic, covalent, metallic and molecular solids. Free electron theory, Fermi sphere, Fermi-Dirac statistics, Ohm's law, limitations of the free electron theory. Electrons in a weak periodic potential (Independent electron model), energy levels in extended, repeat and reduced zone schemes

**Electrical and Magnetic Properties of Solids:** Metals: calculation of density of states, origin of resistivity, weak paramagnetism. Semiconductors: Intrinsic and extrinsic- p and n-types, Hall Effect, Junctions and their applications- metal-metal, metal-semiconductor, semiconductor-semiconductor types and transistors.

**Insulators-** dielectric properties, piezo and inverse piezoelectric effects, ferroelectricity, ferroelectric transitions in  $\text{BaTiO}_3$ , ionic conductivity applications of band theory to  $\text{TiO}$  and  $\text{NiO}$ : Limitations of the Independent electron model, modelling electron correlation.

## UNIT II

**Advanced Magnetochemistry:** Definition of magnetic properties, types of magnetic bodies, Curie equation, Curie's law and Curie-Weiss law. Anisotropy in magnetic susceptibility, diamagnetism in atoms and polyatomic system, Pascal's constants, two sources of paramagnetism, spin and orbital effects, spin-orbit coupling, Lande interval rule, energies of J levels, first order and second order Zeeman effects, temperature independent paramagnetism, simplification and application of van Vleck susceptibility equation, quenching of orbital moment,



magnetic properties of transition metal complexes, low spin, high-spin crossover, magnetic behavior of lanthanides and actinides, magnetic exchange interactions. Molecular magnets, Single Molecule Magnets (SMMs), 3d, 4f and 3d-4f based SMMs. Experimental arrangements for determination of magnetic susceptibility: SQUID.

### UNIT-III

**Dynamics of Atoms in a Solid:** Dispersion curves of an elastic structureless medium, Longitudinal and Transverse modes, Optical and Acoustic modes of a crystal, total vibrational energy of a crystal. Case study of calcite.

**Defects in Solids:** Point defects, Line defects and Plane defects, Stacking faults and grain boundaries.

**Superconductivity:** Superconductivity, Meisner effect, Type I and type II superconductors, Features of superconductors, Frolich diagram, Cooper pairs, Theory of low temperature superconductivity, Junctions using superconductors.

**Phase Transition in Solids:** Definitions, Classification of phase transitions, First and second order phase transitions: Martensitic transition, order-disorder transitions and spinodal decomposition.

### UNIT IV

**Electrochemical aspects of inorganic systems:** Electrochemical synthesis: Special features of electrochemical synthesis compared to conventional synthesis-reaction variables (electrode material, electrode potential, solvent, supporting electrolyte, temperature, agitation) in electrochemical synthesis. Examples of electro-inorganic and electrochemical nanoparticles synthesis with mechanism.

The electrochemical interface between biomolecules, cellular membrane, transmembrane potential, bilayer lipid membranes, electroporation, biological electron transport, electrochemistry of redox enzymes, biological membrane and membrane mimics. Biosensors- NADP, glucose, phenolic. Bioelectroanalysis: Electrolysis and Electrodialysis.

Corrosion and its prevention: use of corrosion inhibitors, use of coatings.

### SUGGESTED TEXT BOOKS

1. Inorganic Electrochemistry: Theory, Practice and Application, Piero Zanello, Royal Society of Chemistry, London, 2007
2. Molecular Electrochemistry of Inorganic, Bioinorganic and Organometallic Compounds  
*Volume 385 of Nato Science Series C*., A.J.L. Pombeiro, J.A. McCleverty, Springer Science & Business Media, 2012
3. Introduction to Magnetochemistry, Alan Earnshaw, Elsevier, 2013
4. Physical principles and applications of magnetochemistry, Sir Shanti Swarupa Bhatnagar, K. N. Mathur, Macmillan and Co., limited, 1935
5. Magnetochemistry, Richard L. Carlin, Springer Science & Business Media, 2012
6. Solid State Chemistry and its Applications, Anthony R. West, 2<sup>nd</sup> Edition, John Wiley & Sons, 2014

## SUGGESTED REFERENCE BOOKS

1. Dynamics of Atoms in Crystals, W.Cochran, Edward Arnold, London,1973.(Pages 24-37)
2. Vibrational Spectroscopy of Solids, P.M.A. Sherwood, University Press, Cambridge, 1972. (Pages: 1-45)
3. Phase Transitions, C.N.R. Rao and K.J. Rao, Cambridge University Press.
4. X-ray Structure determination: Apracticalguide, George H Stoutand Lyle H Jenson, Macmillan Publishing Co.Inc and Collier Macmillan Publishers.
5. Solid State Chemistry: An Introduction, Fourth Edition, Lesley E. Smart, Elaine A. Moore, CRC Press, 2016
6. Electrochemistry of Metal Complexes: Applications from Electroplating to Oxide Layer Formation, Arvydas Survila, John Wiley & Sons, 2015
7. Biological Electrochemistry, Volume 1, Glenn Dryhurst, Elsevier, 2012

| Course Title: Modern Organic Synthesis |                                                                          |                 |                       |
|----------------------------------------|--------------------------------------------------------------------------|-----------------|-----------------------|
| Course Code                            | CHE91DC02304                                                             | Credits         | 4                     |
| L + T + P                              | 3 + 1 + 0                                                                | Course Duration | One Semester          |
| Semester                               | Odd                                                                      | Contact Hours   | 45 (L) + 15 (T) Hours |
| Methods of Content Interaction         | Lecture, Tutorials, Group discussion; self-study, seminar, presentations |                 |                       |

**OBJECTIVE:** Utilise the knowledge of stereochemistry to understand different stereo-controlled chemical reactions and the role of the reagents in organic transformation with their reaction mechanism. Development of knowledge for the rational mechanism-based design of synthetic strategies for novel organic reactions.

### UNIT I

**Chiral substrates controlled asymmetric synthesis:** Stereoselective Nucleophilic addition to carbonyl compounds, 1, 2-asymmetric induction, Cram's rule and Felkin-Anh model, Cyclic Model for 1,2 Asymmetric Induction. Cyclic and acyclic enolates: kinetic vs thermodynamic stability: Alkylations, and aldol reactions.

**Chiral auxiliary controlled asymmetric synthesis: aldol reaction:** Evans approach, Crimmins approach,  $\alpha$ -hydroxylation,  $\alpha$ -alkylation, C-N and C-X-Bond forming reactions.

**Reagent controlled asymmetric synthesis: aldol reaction:** Ian Paterson Approach, 1,2 Asymmetric Induction: Diastereoselective Allylation with Chiral Boron Reagents. Brown allylation, reductions. Chiral catalyst controlled Diastereoselective transformation.

### UNIT II

**Oxidising Reagents:** Metal based and non-metal-based oxidations of (a) **alcohols to carbonyls:** (i) Chromium based Cr(IV) Oxidants: Jones reagent,  $\text{CrO}_3$ , PCC, PDC, Manganese, aluminium, silver, and ruthenium. (ii) **DMSO oxidants:** Moffatt-Pfitzner

Oxidation, swern oxidation, Torrsell oxidation, Parikh-Doering Oxidation, Corey–Kim oxidation, Kornblum Oxidation (iii) **Hypervalent iodine:** IBX, DMP and TEMPO based reagents, and TPAP. (b) **Alkenes to epoxides** (peroxides/per acids based), Sharpless asymmetric epoxidation, Jacobsen epoxidation, Shi epoxidation. (c) **Alkenes to diols** (Manganese, Osmium based), Sharpless asymmetric dihydroxylation, Prevost reaction and Woodward modification, (d) **alkenes to carbonyls with bond cleavage:** Manganese, Osmium, Ruthenium and Lead. (e) **Oxidation of active C-H bonds:** SeO<sub>2</sub>, DDQ, CAN, NBS.

### UNIT III

**Reducing Reagents:** Reduction: (a) **Catalytic hydrogenation** (Heterogeneous: Palladium / Platinum / Rhodium / Nickel etc; Homogeneous: Wilkinson). Noyori asymmetric hydrogenation. (b) Dissolving metal reductions: Li/Na/Ca in liquid ammonia, Sodium, Magnesium, (Birch, Pinacol formation, McMurry, Acyloin formation, (c) **Hydride transfer reagents/ nucleophilic metal hydrides:** from Group III and Group IV in reductions. (i) Al based reagents: LiAlH<sub>4</sub>, DIBAL-H, and Red-Al; NaBH<sub>4</sub>, and its derivatives such as triacetoxyborohydride, L-selectride, K-selectride, Luche reduction; Trialkylsilanes and Trialkylstannane,) (ii) Stereo/enantioselectivity reductions (Chiral Boranes, Corey-Bakshi-Shibata), (iii) **Electrophilic metal hydrides:** AlH<sub>3</sub>, BH<sub>3</sub>

**Coupling reagents for functional groups:** for alcohols, amines and acids: EDCI, DCC, HATU, HOBt, HBTU, HCTU, Yamaguchi lactonization.

### UNIT IV

**I). Protecting Groups:** (i) **Protection of alcohols** as ethers: (a) MOMCl, MEMCl, etc., (b) silyl ether TMSCl, TESCl, TBDPSCl, TIPSCl, TDPSCl, and (c) ester formation: Boc, Cbz. (ii) **Methods for deprotections** of Silyl, Cbz, Boc (ii) **Protection of 1,2-diols and 1,3-diols**, (iii) **Protection of amines:** by benzyloxy carbonyl, *t*-butyloxycarbonyl, fmoc and triphenyl methyl groups. (iv) Protection of carbonyls by acetal, ketal and thiol acetal (Umpolung) groups. (v) Protection of carboxylic acids by ester.

**II) Organic Retrosynthesis and its application to natural product synthesis:** Disconnection Approach: An introduction to synthons, retrons and synthetic equivalents, Functional group transposition, Functional group inter-conversions, disconnection approach, the importance of the order of events in organic synthesis, one group and two group C-X disconnections, one group C-C and two group C-C disconnections, illogical disconnections, linear and convergent synthesis. Chemoselectivity, regioselectivity, reversal of polarity (umpolung).

**Synthesis of some complex molecules:** synthetic routes based on retrosynthetic analysis.

### SUGGESTED TEXT BOOKS

1. F. A. Carey and R. I. Sundberg, Advanced Organic Chemistry, Part A and B, 5<sup>th</sup> Edition, Springer, 2009.
2. M. B. Smith, Organic Synthesis, 2<sup>nd</sup> Edition, 2005
3. S. Warren, Organic Synthesis, The disconnection Approach, John Wiley & Sons, 2004.

4. I. Ojima, Catalytic Asymmetric Synthesis, 2<sup>nd</sup> edition, Wiley–VCH, New York, 2000.
5. W. Carruthers, Modern Methods of Organic Synthesis, Cambridge University Press, 1996.
6. J. Clayden, N. Greeves, S. Warren and P. Wothers, Organic Chemistry, Oxford University Press, 2001.
7. R. Noyori, Asymmetric Catalysis in Organic Synthesis, John Wiley & Sons, 1994.
8. Nasipuri D. Stereochemistry of Organic Compounds, New Age Publications.
9. Protective groups in organic synthesis 4<sup>th</sup> Ed. 2007 - Greene & Wuts

### SUGGESTED REFERENCE BOOKS

1. The Logic of Chemical Synthesis by E. J. Corey & X-M. Cheng
2. Classics in Stereoselective Synthesis by Carreira, E. M.; Kvaerno, L, Wiley VCH, 2009
3. Classics in Total Synthesis by K. C. Nicolaou & E. J. Sorensen, VCH, 1996.
4. Classics in Total Synthesis II, K. C. Nicolaou & S. A. Snyder, VCH, 2003
5. J. Tsuji, Palladium Reagents and Catalysts, New Perspectives for the 21<sup>st</sup> Century, John Wiley & Sons, 2003.
6. L. Kuerti and B. Czako, Strategic Applications of named Reactions in Organic Synthesis, Elsevier Academic Press, 2005
7. Protective Groups in Organic Synthesis 3<sup>rd</sup> Ed - Peter G. M. Wuts
8. Gawley R. E. and Aube J. Principles of Asymmetric Synthesis, Pergamon.
9. Eliel E. L. Stereochemistry of Organic Compounds, Wiley.

| <b>Course Title: Applied Electrochemistry</b> |                                                                          |                        |                          |
|-----------------------------------------------|--------------------------------------------------------------------------|------------------------|--------------------------|
| <b>Course Code</b>                            | <b>CHE91DC03404</b>                                                      | <b>Credits</b>         | 4                        |
| <b>L + T + P</b>                              | 3 + 1 + 0                                                                | <b>Course Duration</b> | One Semester             |
| <b>Semester</b>                               | Odd                                                                      | <b>Contact Hours</b>   | 45 (L) + 15 (T)<br>Hours |
| <b>Methods of Content Interaction</b>         | Lecture, Tutorials, Group discussion; self-study, seminar, presentations |                        |                          |

### Course Objectives

- To acquaint students with applications of electrochemistry in daily life
- To make students proficient in advanced level electroanalytical methods such as polarography and cyclic voltammetry
- To make students aware of various methods of electrochemical energy conversion and storage.
- To make students learn techniques of electroplating and metal finishing
- To impart knowledge about corrosion and its prevention

**Learning Outcomes:** After completion of the course the learners will be able to:

- Apply the concept of polarography and voltammetry to solve problems in daily life
- Explain the construction and working of various types of batteries and fuel cells
- Distinguish between various electroplating techniques and use it for different purposes
- Use electrochemical techniques to prevent corrosion

## UNIT-I

### APPLIED ELECTROCHEMISTRY

**Electroanalytical methods:** Voltammetry: Definition, concentration polarization, ideal and non-ideal polarized electrodes, Faradaic and non-faradaic currents.

**Polarography-** Construction of dropping mercury electrode (DME), advantages and limitations. Principle of normal dc polarography, half-wave potential, and qualitative analysis using polarograms. Types of currents obtained at a DME. Ilkovic equation, factors affecting diffusion controlled current, quantitative analysis based on Ilkovic equation. Current- potential relation for ac cathodic wave, anodic wave and composite wave, test for the reversibility of a process at DME, factors that set the sensitivity and selectivity limits in normal dc polarography.

**Advanced polarographic techniques:** Fast polarography, normal pulse polarography, differential pulse polarography, ac polarography.

**Stripping voltammetry:** Hanging drop mercury electrode (HDME), principles and applications of cathodic and anodic stripping voltammetry.

**A: Cyclic voltammetry:** Principle, experimental setup, quantitative analysis. Diagnostic criteria for reversible, quasi- reversible and irreversible processes. Study of coupled chemical reactions like  $E_R C_R$ ,  $C_R E_R$  and  $E_R C_I E_R$ .

**B.Chronomethods:** Basic concepts, methodology and applications of chronoamperometry, chronopotentiometry and chronocoulometry.

**C. Hydrodynamic electrodes:** Construction and use of rotating disc and rotating ring disc electrodes in the electrochemical studies.

**D.Membrane electrodes:** Ion-selective membrane electrodes-construction and applications of solid state and liquid membrane electrodes, ion selective field effect transistor and Molecular (gas) sensing probes.

**E.** Problems solving.

## UNIT-II

### Electrochemical energy conversion and storage

**Batteries:** History and basics, classification, characteristics with units-voltage, current, capacity, electricity storage density, energy density, power density, energy efficiency, cycle life, shelf life. Primary batteries: Construction, reactions and uses of Leclanche dry cell, alkaline Leclanche cell, zinc- silver oxide cell.

**Secondary batteries:** Construction, working (charge-discharge reactions), applications advantages and of Pb-acid and Ni-Cd batteries.

**Hybrid Batteries: Metal-air batteries-**meaning, Zn-air battery, Fe-air battery, Charging of metal- air battery, Metal oxide-hydrogen / hydride batteries, advantages and limitations of

these cells *Lithium batteries*: Primary and secondary lithium battery, Li-ion battery and Lithium ion- polymer battery.

**Electrochemical super capacitors**: comparative meaning of capacitor, electrolytic (super) capacitor and ultra-capacitors, materials for construction, applications, advantages and limitations.

**Fuel cells**: Energy efficiency of electrochemical and thermal conversion (Carnot limitation). Definition of fuel cell, classification. Fuel cell efficiency- thermodynamic, electrochemical, practical efficiency. Electrode (anode and cathode) mechanism of fuel cell, Brief description on construction, working principle and applications of each type fuel cells. An account of electrocatalysts, proton exchange membrane (PEM) fuel cells and direct methanol fuel cell. Problems solving.

### UNIT-III

**Surface Modification techniques (Metal finishing)**: Definition, important processes of metal finishing, technological importance of metal finishing. *Electroplating*: Definition, theory and mechanism of electroplating, effect of plating variables on the properties of electrodeposits, comparative account of complexing and non-complexing baths (general treatment), additives in the platingbath and their significance.

**Metallic coating**: Preparation of substrate surface, electroplating of Cu and Cr. Applications of Au and Ag platings.

**Solar selective coatings**: Characteristics, methods of preparation and applications.

**Techniques of electroplating**: Galvanizing, Anodizing, Phosphating, Chromating. Electroless plating: Definition, advantages over electroplating, pretreatment of substrates, an account of electroless plating of Ni including applications.

### UNIT-IV

#### Corrosion and its Prevention

Introduction, dry and wet corrosion, theories and mechanisms of wet (electrochemical) corrosion, thermodynamic aspects of corrosion, kinetic aspects- determination of rates of corrosion by linear polarization, Tafel extrapolation and impedance techniques. Factors influencing the rate of corrosion-metal and environmental.

Methods of corrosion prevention: Cathodic protection, anodic protection, use of corrosion inhibitors, use of organic coatings.

**Passivity**: Definition, current potential diagram, characteristics of passivity, theory and mechanism of passivation, flade potential, transpassivity, Use of ellipsometric technique in the study of passivating films. Problems solving

#### SUGGESTED TEXT BOOKS

1. Modern Electrochemistry, Vol.1, 2 A and 2 B by Bockris and Reddy, Plenum, N.Y (2000).
2. Polarography and Allied Techniques by V Suryanarayana Rao, Universities Press (India) Pvt. Ltd., Hyderabad (2002).
3. Basic concepts of Analytical Chemistry by SM Khopkar, New Age International Publishers, third edition, New Delhi, 2008.

4. Electrochemical Methods- Fundamentals and Applications, 2<sup>nd</sup> Edn, by A J Bard and LR Faulkner, John Wiley & Sons Inc., New York (2001).
5. Chemical and Electrochemical Energy systems by Narayan and Viswanathan, Hyderabad, Universities Press (India) Pvt. Ltd., Hyderabad (2002).
6. Understanding Batteries, RM Delland DAJ Rand, 2001.6. Fuel cells and their applications, Karl kordesh, gunter, Simader, VCH-Weinheim, Cambridge, 1996.
7. Fundamentals of electrochemical deposition, Milan Paunovic and Mordechay Schlesinger, Wiley-interscience publications, New York, 199
8. Electrodeposition and Corrosion Control, J.M.West, J. Wiley W. Revie (ed.): Corrosion Handbook, Electrochemical Society Series, John Wiley and Sons (2000)
9. Electrochemistry and corrosion science, Nestor Perez, Springer pvt. Ltd., 2004
10. Principles and Prevention of Corrosion, D. A. Jones, Macmillan Publ.Co. (1996).
11. Bioelectrochemistry: Fundamentals, experimental techniques and application, P. N. Bartlett, Wiley & Sons (2008).
12. Synthetic organic Electrochemistry by A MFry, 2<sup>nd</sup> Edn, Wiley 1989.

| <b>Course Title: Inorganic Reaction Mechanism, Organometallics and Advance Bioinorganic Chemistry</b> |                                                                          |                        |                       |
|-------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------|------------------------|-----------------------|
| <b>Course Code</b>                                                                                    | <b>CHE91DC01404</b>                                                      | <b>Credits</b>         | <b>4</b>              |
| <b>L + T + P</b>                                                                                      | 3 + 1 + 0                                                                | <b>Course Duration</b> | One Semester          |
| <b>Semester</b>                                                                                       | Odd                                                                      | <b>Contact Hours</b>   | 45 (L) + 15 (T) Hours |
| <b>Methods of Content Interaction</b>                                                                 | Lecture, Tutorials, Group discussion; self-study, seminar, presentations |                        |                       |

#### **Course Objectives**

- To develop comprehensive understanding of reaction mechanism involving metal complexes
- To make students understand the role of organometallics in industrial catalysis and medicine
- To impart knowledge of structure and functions of metalloproteins
- To make the students understand the mechanism of metal ion transport across the cell membrane and discuss the toxicity of metals
- To impress upon the students the versatility and efficiency of the oxygen transport systems and nitrogen fixation in biology

#### **Learning Outcomes**

- After completion of the course the learners will be able to:
- Explain the electron transfer processes involving metal complexes
- Analyse the role of organometallics in catalysis and medicine and design new ones
- Analyse the structure and functions of metalloproteins
- Elaborate the oxygen transport system in various biosystems
- Illustrate the detoxification scheme for heavy metals and chelation therapy

## UNIT I

**Reaction mechanism-** Substitution in square planar complexes-factors affecting substitution, mechanism of substitution reaction-associative, dissociative, interchange associative, interchange dissociative, trans-effect, Application of trans-effect in the synthesis of complexes. Mechanism of ligand substitution in octahedral complexes- kinetics, factors affecting substitution in octahedral complexes: Leaving group, chelate and metal effects. Examples of Labile, inert, stable and unstable complexes. Mechanism of isomerization reactions in octahedral complexes with and without bond breaking.

Electron transfer reactions, complementary and non-complementary, outer sphere electron transfer-Marcus's equation, Inner sphere electron transfer- one and two electron transfer, use of electron transfer reactions for the synthesis of complexes.

## UNIT II

Synthesis, Structure and Bonding of metal carbonyl complexes, carbonylate ions, metal carbonyl hydride complexes, Vasaka's complex, Nitrosyl complexes, Isoelectronic and isolobal fragments, Fischer and Schrock carbene and carbyne. Metal alkene, alkyne and carbide complexes, Allyl and pentadienyl complexes, Metallocene.

Reactivity and Catalysis: Oxidative addition and Reductive elimination, Agostic interaction, Insertion and Elimination reaction, Nucleophilic and electrophilic attack of coordinated ligands, Wilkinson's catalyst, Homogeneous catalysis: Hydrogenation, asymmetric hydrogenation; hydroformylation-cobalt and modified catalysts, Wacker process-acetaldehyde from ethylene; Monsanto acetic acid process, Olefin metathesis; water gas shift reaction; Fischer Tropsch Process; Ziegler Natta catalysis, medicinal applications of organometallic complexes. Oxidative addition, reductive elimination, isomerisation, migratory insertion reactions.

## UNIT III

**Metalloproteins:** Introduction, Iron protein: Heme, Protoporphyrin IX, Structure and functions of haemoglobin and myoglobin, Cooperativity, Perutz mechanism, dioxygen binding, Bohr Effect, Hill equation, non-porphyrin systems- hemerythrin and hemocyanin. Cytochromes, Mitochondrial flow of electrons from NADH to oxygen, cytochrome C, Cytochrome C oxidase. Iron sulphur protein: Rubredoxins, Ferredoxins-  $2\text{Fe}-2\text{S}$ , Rieskecenters,  $3\text{Fe}-4\text{S}$ ,  $4\text{Fe}-4\text{S}$ ,  $8\text{Fe}-8\text{S}$ .

**Metalloenzymes:** Structure and reactivity-Zinc enzymes: carboxypeptidase, carbonic anhydrase, alcohol dehydrogenase. Cu enzyme: superoxide dismutase. Mo enzyme: Xanthine oxidase, nitrate reductase. Fe enzymes: catalase, peroxidase, acid phosphate and cytochrome P-450. Vitamin  $\text{B}_{12}$ : Coenzyme:  $\text{B}_{12\text{r}}$ ,  $\text{B}_{12\text{s}}$ , biochemical functions of cobalamins; Biomethylation.

## UNIT IV

**Photosynthesis and nitrogen fixation:** Nitrogenase: structural aspects and functions, nitrogen fixation. Photosynthesis: Chlorophyll- structural features, role of  $\text{Mg}^{2+}$ , Z scheme of photosynthesis-PS-I and PS-II.

**Metals in transport, fixation and medicine:**  $\text{Na}^+/\text{K}^+$  transport across cell membranes, ionophores,  $\text{Na}^+/\text{K}^+$  pump. Iron storage and transport: siderophores, transferrin and ferritin. Metal ion deficiency and treatment (Fe, Zn, Cu, Mn); toxicity of Fe, Cu, Heavy Metals-As,



Hg, Pb and Cd; detoxification; chelation therapy; Biological roles of Ca: Binding sites of  $\text{Ca}^{2+}$  in proteins, importance of  $\text{Ca}^{2+}$  in muscle contraction and in blood clotting process. Metal complexes as anticancer and antiarthritic drugs.

### SUGGESTED TEXT BOOKS

1. The organometallic chemistry of transition metals; R. H. Crabtree; John Wiley, 6<sup>th</sup> edition.
2. Catalytic chemistry; B. C. Gates; John Wiley and sons, 1992.
3. Applied Organometallic chemistry and catalysis; Robin Whyman, Oxford Chemistry Primers, 2001
4. Reaction mechanism of inorganic and organometallic systems; J. B. Jordon, Oxford University Press 2<sup>nd</sup> edition, 1998.
5. Principles of Bioinorganic Chemistry; S. J. Lippard and J. M. Berg; Panima Pub. Corporation 1997.
6. Bioinorganic Chemistry - Inorganic Elements in the Chemistry of Life, W Kaim, 2<sup>nd</sup> Edition,
7. Wiley Inorganic Chemistry, 3<sup>rd</sup> Edition; Gary. L. Miessler and Donald. A. Tarr (2007).
8. Bio-inorganic chemistry, I. Bertini, H. B. Gray, S. J. Lippard and J. S. Valentine, Viva Books Pvt. Ltd 1998.

### SUGGESTED REFERENCE BOOKS

1. F. A. Carey G. Wilkinson, C. A. Murillo and M. Bochmann, Advanced Inorganic Chemistry, Wiley Interscience, 2003.
2. C. E. Housecroft and A. G. Sharpe, Inorganic Chemistry, Prentice Hall, 2005.
3. Organometallics; Vol 1 & 2; M. Bochmann, Oxford Chemistry Primers, Oxford University Press, 1994.
4. Inorganic Chemistry; K. F. Purcell and J. C. Kotz, Saunders Company, 1977.

| Course Title: Chemistry of Biomolecules |                                                                          |                 |                       |
|-----------------------------------------|--------------------------------------------------------------------------|-----------------|-----------------------|
| Course Code                             | CHE91DC02404                                                             | Credits         | 4                     |
| L + T + P                               | 3 + 1 + 0                                                                | Course Duration | One Semester          |
| Semester                                | Odd                                                                      | Contact Hours   | 45 (L) + 15 (T) Hours |
| Methods of Content Interaction          | Lecture, Tutorials, Group discussion; self-study, seminar, presentations |                 |                       |

**OBJECTIVE:** Acquire foundational knowledge of the chemistry of life. Examine the relationship between the structure and function of biological molecules. And apply this knowledge in research and development in the area of Biomedical Analysis as well as Biomedical Methods and Technology.

## UNIT I

**Amino acids and Peptide:** Amino acids, structural features, optical activity, essential and non-essential amino acids, iso-electric point, synthesis and chemical properties of  $\alpha$  amino acids. Peptides: Structure and synthesis, Protecting and activating groups, solid phase peptide synthesis.

**Proteins:** classifications, primary, secondary, tertiary and quaternary structure of proteins, glycoproteins, denaturation and folding.

**Enzyme:** Nomenclature and classification, Remarkable properties of enzymes like catalytic power, specificity and regulation, Proximity effects and molecular adaptation, Chemical and biological catalysis. Mechanism of enzyme action: Fischer's lock and key and Koshland's induced fit hypothesis, concept and identification of active site by the use of inhibitors affinity labeling and enzyme modification by site directed mutagenesis.

**Receptors:** Type of receptors, Receptor-ligand interaction, Enzymes, agonists, partial agonist, inverse agonists, neutral antagonists and antagonist

## UNIT II

**Coenzyme:** Cofactors as derived from vitamins, coenzymes, prosthetic groups, and apoenzymes. Structure and biological functions of coenzyme A, thiamine pyrophosphate pyridoxal phosphate,  $\text{NAD}^+$ ,  $\text{NADP}^+$ , FMN, FAD, Lipoic acid, vitamin  $\text{B}_{12}$ . Mechanisms of reactions catalyzed by the above co-factors.

**Nucleosides, Nucleotides and Nucleic Acids:** Nucleosides, Nucleotides, Elementary idea of nucleic acids and complementary base pairing, ATP: The Carrier of Chemical Energy, Phosphodiester bonds, Oligonucleotides and polynucleotides, Nucleic acids, Secondary and tertiary structures, the double helix

**Lipids:** Classification and biological importance of fatty acids and lipids, stereochemical notation in lipids, chemical synthesis of phospholipids and glycolipids, properties of lipid aggregates, micelles, bilayers, lysosomes and biological membranes.

## UNIT III

**Carbohydrates:** Types of naturally occurring sugars, deoxy sugars, amino sugars, branched chain sugars, sugar methyl ethers and acid derivatives of sugars, polysaccharides of industrial and biological importance, dextran, chemistry of sialic acids, cell-cell recognition and blood group substances.

## UNIT IV

**Concept of Energy in Biosystems:** Introduction to Metabolism (catabolism, anabolism), ATP: the universal currency of cellular energy, ATP hydrolysis and free energy change. Conversion of food into energy. Outline of catabolic pathways of Carbohydrate- Glycolysis, Fermentation, Krebs cycle. Overview of catabolic pathways of Fats and Proteins. Interrelationships in the metabolic pathways of Proteins, Fats and Carbohydrates.

## SUGGESTED TEXT BOOKS

1. Dugas, H. & Penney, C. Bioorganic Chemistry: A Chemical Approach to Enzyme Action Springer-Verlag (1989).
2. Saenger, W. Principles of Nucleic Acid Structure Springer-Verlag (1984).

3. Sinden, R. P. DNA Structure and Function Academic Press (1994).

### SUGGESTED REFERENCE BOOKS

1. Crowe J and Bradshaw T. (2010) Chemistry for the biosciences- The essential concepts. Oxford University Press, 2<sup>nd</sup> ed.
2. Principles of Biochemistry 6<sup>th</sup> edition, 2006 - Jeremy M. Berg, John L. Tymoczko and Lubert Stryer (W.H. Freeman & Co.)
3. Lehninger Principles of Biochemistry 5<sup>th</sup> edition, 2008 - Nelson, D. L. and M. M. Cox. (W. H. Freeman & Co.).
4. Outlines of Biochemistry 5<sup>th</sup> edition 2001- Conn, E.E., Stumpf, P. K. Bruening, G. and Doi, R.H. (John Wiley and Sons).
5. Harper's Illustrated Biochemistry - R.K. Murray et al. (McGraw Hill)

| Course Title: Advanced Photochemistry |                                                                          |                 |                       |
|---------------------------------------|--------------------------------------------------------------------------|-----------------|-----------------------|
| Course Code                           | CHE91DC03504                                                             | Credits         | 4                     |
| L + T + P                             | 3 + 1 + 0                                                                | Course Duration | One Semester          |
| Semester                              | Odd                                                                      | Contact Hours   | 45 (L) + 15 (T) Hours |
| Methods of Content Interaction        | Lecture, Tutorials, Group discussion; self-study, seminar, presentations |                 |                       |

### Course Objectives

- To further enhance the understanding of photochemistry
- To make students learn the physicochemical properties of electronically excited state
- To acquaint students with the environmental effects on absorption and emission spectra
- To develop an understanding of different types of photochemical reactions
- To impart knowledge about emerging topics such as photo-electrochemistry, photovoltaics and photo-splitting of water

**Learning Outcomes:** After completion of the course the learners will be able to:

- Draw Electronic, vibrational, rotational energies-potential energies diagram and explain the photochemical processes
- Distinguish between photoluminescence, electroluminescence and chemiluminescence
- Discuss the effect of solvents on absorption and emission spectra
- Analyze a photochemical reaction, determine the rate constant and photochemical quantum yield
- Discuss the role of photochemical processes in photovoltaics and generation of hydrogen energy

### UNIT I

Importance of Photochemistry, Laws of Photochemistry: Grothus –Draper Law, Stark-Einsteins Law, Laws of light absorption, Quantum yield and numerical problems. Photochemistry and spectroscopy, units and dimensions. Electronic energy states of atoms,

term symbols for atoms, energy levels for the electronic configuration of carbon and oxygen illustrating spin orbit coupling and Hunds rules, inverted multiplets as applied to simple atoms and also for inner transition metals, Laporte's selection rules. Physicochemical Properties of electronically excited molecules: Nature of changes on electronic excitation: acidity, dipole moment, redox potentials etc. Fates of excited species, Electronic, vibrational, rotational energies-potential energies diagram. Shapes of absorption band and Franck Condon principle.

## UNIT II

Quantum mechanical formulation of Franck Condon, crossing of potential energy surfaces, Non crossing rule of Teller for potential energy surface. Emission spectra, fluorescence and phosphorescence.

Environmental effect on absorption and emission spectra, solvent red shift and blue shift in absorption spectra. Experimental techniques to determine the intermediates in photochemical reactions.

Classification of photochemical reactions, Rate constants and life times of reactive energy state Effect of light intensity on the rate of photochemical reaction Photo-fragmentation of photo dissociation-Gas phase photolysis.

## UNIT III

Photosensitized reaction, photofragmentation in liquid phase, photodegradation of polymers, Isomerization and other rearrangement reactions, Atmospheric photochemistry.

### **Some current topics in photochemistry:**

**Semiconductors:** Bonding and conductivity, mechanism of conductivity, energy bands in semiconductors, impurity semiconductors.

## UNIT IV

**Photo voltaic effect:** p-n junction solar cells, silicon cells, GaAs solar cells, schottky barrier solar cells.

**Photo-electrochemistry:** Introduction, efficiency of conversion of light to chemical and electrical energy, frequently measured quantities. Photo-splitting of water using colloidal suspensions Photocatalysis: Photocleavage of waste which are environmentally hazardous by using TiO<sub>2</sub>, Photooxidation and photoreduction reactions.

## SUGGESTED BOOKS

1. Fundamentals of photochemistry, K.K. Rohatgi Mukherjee, Wiley Eastern Limited (1986)
2. Photochemistry, Carol E Wayne and Richard P Wayne, Oxford University Press (1996)
3. Introduction to Semiconductor Materials and devices M S Tyagi, John Wiley and sons (1991)
4. Organic Photochemistry, J. M. Cozen and B. Halton, Cambridge University Press (1<sup>st</sup> Edition) 1974
5. Molecular Reactions and Photochemistry, C H Deputy and D S Chapman, Prentice Hall India, New Delhi (1<sup>st</sup> Edition), 1972.

## SUGGESTED REFERENCE BOOKS

1. Principles of Fluorescence Spectroscopy, 3<sup>rd</sup> Ed., J. R. Lakowicz, Springer, New York, 2006.
2. Fundamentals of Photoinduced Electron Transfer, G. J. Kavarnos, VCH publishers Inc., New York, 1993.
3. Molecular Fluorescence: Principles and Applications, B. Valeur, Wiley-VCH Verlag GmbH, Weinheim, 2002.
4. Modern Molecular Photochemistry of Organic Molecules, N. J. Turro, V. Ramamurthy, J. C. Scaiano, University Science, Books, CA, 2010.
5. Photochemical Synthesis, I. Ninomiya, T. Naito, Academic Press, New York, 1989.

## **FOURTH SEMESTER (EVEN SEMESTER)**

| <b>Course Title: Surface Phenomena, Colloids and Statistical Thermodynamics</b> |                                                                          |                        |                       |
|---------------------------------------------------------------------------------|--------------------------------------------------------------------------|------------------------|-----------------------|
| <b>Course Code</b>                                                              | <b>CHE92DC03604</b>                                                      | <b>Credits</b>         | 4                     |
| <b>L + T + P</b>                                                                | 3 + 1 + 0                                                                | <b>Course Duration</b> | One Semester          |
| <b>Semester</b>                                                                 | Even                                                                     | <b>Contact Hours</b>   | 45 (L) + 15 (T) Hours |
| <b>Methods of Content Interaction</b>                                           | Lecture, Tutorials, Group discussion; self-study, seminar, presentations |                        |                       |

### **Objective:**

- To impart knowledge of surface structure and skills in analysing the adsorption phenomena through different types of isotherms, eg, Gibbs, BET, Langmuir etc
- To make the students understand colloids and related phenomena and correlate it with examples in daily life
- To equip the students with necessary knowledge and skills in Statistical Thermodynamics, and non-equilibrium thermodynamics

**Learning Outcomes:** After completion of the course the learners will be able to:

- Determine the binding affinity of analyte on a surface using Langmuir or BET isotherms
- Design colloidal systems with enhanced stability and use it for solving problems in daily life
- Write partition functions for rotational, vibrational motion or electron dynamics in molecules

### **Unit-I**

**Surface Phenomena:** Main features of surfaces, steps, kinks, terrace, vacancy, adatom; Types of adsorption isotherms, Effect of temperature on adsorption, Mechanical adsorption, Estimation of surface area using BET equation, Gibbs adsorption isotherm and its significance, Freundlich isotherm, Langmuir isotherm, Dubinin-Radushkevich isotherm, Temkin isotherm; Surface tension and surface energy, Pressure difference across curved

surface (Laplace equation), Vapour pressure of droplets (Kelvin equation), Surface film on liquids (electro-kinetic phenomena), Catalytic activity of surfaces.

### Unit-II

**Colloids:** types of colloids, relationship with interface, contact angle & wetting, Brownian motion, sedimentation, adsorption from solution, micellization & self-assembly, Intermolecular forces & introduction to the electric double layer, zeta-potential, coagulation and flocculation, micellar catalysis. Host- guest chemistry.

### Unit-III

**Statistical Thermodynamics:** Introduction: Concept of ensembles, partition functions and distributions, microcanonical, canonical and grand canonical ensembles, canonical and grand canonical partition functions, Boltzmann, Fermi-Dirac and Bose-Einstein distributions. Gibbs paradox and Sackur – Tetrode equation. Concept of thermal wavelength. Molecular partition functions – translational, rotational, vibrational, electronic, nuclear. Equipartition theorem and its validity. Problems and their Solutions. System of interacting molecules – Imperfect gas. Specific heat of electron gas, Bose condensation.

### Unit-IV

**Non-equilibrium Thermodynamics:** Thermodynamic criteria for non-equilibrium states- Phenomenological Laws and Onsager's Reciprocity relations, Coupled and Non-coupled reactions, Entropy production and entropy flow. Electro- kinetic Phenomenon.

**Introductory Computational Chemistry:** Introduction to the computational chemistry and molecular modelling, Coordinate systems, Concept of 2D and 3D structure, molecules, Surfaces, Molecular energetic profile, Brief idea about the computational softwares for drawing, visualization and simulation of small and large molecules. Basic concept of Cheminformatics, 3D-Structure file system and Databases.

### SUGGESTED TEXT BOOKS

1. D. Chandler, Introduction to Modern Statistical Mechanics, Oxford University Press, 1987.
2. A Textbook of physical Chemistry Vol- 4 and 5, K. L. Kapoor 5<sup>th</sup> edition McGraw Higher Ed (2015).
3. Thermodynamics, by Rajaraman and Kuriacose, East-West Press, (1986).
4. Statistical Thermodynamics, M. C. Gupta (Wiley Eastern Ltd.) 1993.
5. Elementary Statistical Thermodynamics, N. D. Smith, Plenum Press, NY, (1982).
6. Elements of Classical and Statistical Thermodynamics, L. K. Nash, Addison-Wiley (1979).
7. Thermodynamics, Statistical Thermodynamics and Kinetics by Thomas Engel & Philip Reid, Pearson Education inc. (2007).
8. An Introduction to Interfaces & Colloids, J.C. Berg, World Scientific (2010).
9. Colloids and Interfaces in Life Sciences and Bionanotechnology, W. Norde, Taylor & Francis (2011)
10. Adsorption: Fundamental Processes and Applications, Mehrorang Ghaedi, Academic Press (2021).

**REFERENCE BOOKS:**

1. Introduction to Adsorption, Chi Tien, Elsevier Science (2018)
2. Colloids and Colloid Assemblies, Frank Caruso, Wiley (2007)
3. Structure and Functional Properties of Colloidal Systems, Roque Hidalgo-Alvarez, Taylor and Francis (2017)

| <b>Course Title: Scientific literature Survey and Dissertation Work</b> |                                                                            |                        |              |
|-------------------------------------------------------------------------|----------------------------------------------------------------------------|------------------------|--------------|
| <b>Course Code</b>                                                      | <b>CHE92DC05008</b>                                                        | <b>Credits</b>         | 8            |
| <b>L + T + P</b>                                                        | 0+ 0 + 16                                                                  | <b>Course Duration</b> | One Semester |
| <b>Semester</b>                                                         | Even                                                                       | <b>Contact Hours</b>   |              |
| <b>Methods of Content Interaction</b>                                   | Project Work (including experiments, dissertation, presentation, and viva) |                        |              |

**OBJECTIVE:** To introduce students to research in various areas of chemistry by engaging them to carry out a project under the supervision of a faculty for two semesters during the third and fourth semesters.

Candidate will be given a topic of **project at the start of semester III**. The candidate is expected to collect relevant literature, read research articles, make a comprehensive review and make a short presentation based on the literature and the proposed plan of work within 1<sup>st</sup> month of semester IV and it is expected from the students to start their project from the first day of semester IV. A comprehensive report of literature survey and research output have to made and then a seminar presentation and group viva/defence will be conducted at the end of semester IV.

or

**\*\*\*\*Following two courses (4+4 credits) are only those students who don't opt Scientific literature Survey and Dissertation Work (8 credits)**

| <b>Course Title: Scientific literature Survey and Scientific Socially Responsible Activities</b> |                                                                                                                                                                               |                        |              |
|--------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------|--------------|
| <b>Course Code</b>                                                                               | <b>CHE92DC06004</b>                                                                                                                                                           | <b>Credits</b>         | 4            |
| <b>L + T + P</b>                                                                                 | 0 + 0 + 8                                                                                                                                                                     | <b>Course Duration</b> | One Semester |
| <b>Semester</b>                                                                                  | Even                                                                                                                                                                          | <b>Contact Hours</b>   |              |
| <b>Methods of Content Interaction</b>                                                            | (a)Literature Survey, Seminar, Presentation and Viva<br>(b)Scientific activities at societal interface (under Unnat Bharat, Swachh Bharat or any such govt-announced schemes) |                        |              |

- (a) Candidate will be given a research topic during the first week of semester-IX. The candidate is expected to carry out literature survey, read research articles, make a comprehensive review and give a seminar presentation where they have to show their understanding on the subject and suggest some alternative solution to problems. Seminar presentation and group viva/defence will be conducted at the end of semester-X.

- (b) Students will be assigned a task which may involve field work and collecting data. The students will then suggest scientific solutions to the problem and the ways to implement them. This work has to be carried out at societal interface under the government-announced schemes such as Swachh Bharat, Unnat Bharat, Samrt Cities, etc. At the end of the work, student will submit a report and give a presentation based on which evaluation will be done.

| <b>Course Title: Basics of Chemical Education</b> |                                                                          |                        |                          |
|---------------------------------------------------|--------------------------------------------------------------------------|------------------------|--------------------------|
| <b>Course Code</b>                                | <b>CHE92DC07004</b>                                                      | <b>Credits</b>         | <b>2+2</b>               |
| <b>L + T + P</b>                                  | 2 + 0 + 2                                                                | <b>Course Duration</b> | One Semester             |
| <b>Semester</b>                                   | Even                                                                     | <b>Contact Hours</b>   | 45 (L) + 15 (T)<br>Hours |
| <b>Methods of Content Interaction</b>             | Lecture, Tutorials, Group discussion; self-study, seminar, presentations |                        |                          |

### **Course Objectives**

- To acquaint students with the fundamentals of formal and informal chemical education
- To impart knowledge and skills for the development of teaching process based on student's conception
- To introduce the concept of teaching and learning at school and undergraduate level aspects
- To make students aware of device opportunities in chemical education

**Learning Outcomes:** After completion of the course the learners will be able to:

- Develop course curriculum for school and undergraduate level
- Apply the effective practices in teaching chemistry
- Discuss the relevance of local and global perspective of chemical education.
- Write the research-based projects based on social and economic needs

### **Unit-I**

Informal chemical education: Introduction, Differences between formal and informal chemical education, Strands of learning of chemistry, Landscape of informal chemical education, Modes of informal education in the context of chemistry, Opportunities for chemistry in informal education.

Human activity in chemistry education, learning and teaching chemistry. Learner's scientific ideas and mis-conceptions. Identifying and designing curriculum to meet learners need. Perspective on the school and undergraduate level chemistry curriculum. Establish connection between local chemistry curriculum and global trends. Effective practices in teaching chemistry.

### **Unit-II**

Teaching variety of media for chemical education, appropriateness of a media, Phenomena-oriented and Inquiry-Based Network Concept (PIN-Concept) in chemical



education. Structure oriented approach in chemical education. Social and economic dimensions relevant chemical education.

Chemistry Education Research for teaching strategies and Design of curriculum. Research of problem solving in chemistry. Research based instructional materials. Use of authentic text and materials. Strategies for generation of interdisciplinary research ideas for school level and undergraduate level chemistry course curriculum.

### UNIT III -Practice

1. Analyses students' difficulties and misconceptions in chemistry
2. Develop methods for effective learning of chemistry.
3. Development of inquiry-based instructional materials
4. Designing problems in theoretical areas with emphasis on context and conceptual understanding

### UNIT IV-Practice

1. Original educational laboratory experiments at both the undergraduate and high school level
2. Enhancement of learning with computer-driven technology
3. Reviews of instrumentation commonly employed in educational laboratory settings
4. Studies and evaluations of educational laboratory teaching methods
5. Non-traditional (e.g., online) educational laboratory experimentation and methods and Laboratory and Classroom demonstrations

### SUGGESTED TEXT BOOKS

1. Chemistry Education: Best Practices, Opportunities and Trends *Edited by* Javier Garcia-Martinez and Elena Serrano-Torregrosa 2015 Wiley-VCH Verlag GmbH & Co.
2. Essentials of Chemical Education: Hans-Dieter Barke, Gunther Harsch, Siegbert Schmid Translated by Hannah Gerdau, Springer, ISBN 978-3-642-21755-5.
3. Creative Chemists: Strategies for Teaching and Learning, Advances in Chemistry Education Series, Simon Rees, Douglas Newton, ISBN 978-1-78801-511-0.
4. Relevant Chemistry Education: From Theory to Practice, Ingo Eilks, AviHofstein, Springer, 22-Jul-2015.  
<http://www.springer.com/us/book/9789463001755>

| Course Title: Chemistry of Materials |              |                 |                       |
|--------------------------------------|--------------|-----------------|-----------------------|
| Course Code                          | CHE92DC01504 | Credits         | 4                     |
| L + T + P                            | 3 + 1 + 0    | Course Duration | One Semester          |
| Semester                             | Odd          | Contact Hours   | 45 (L) + 15 (T) Hours |

|                                       |                                                                          |
|---------------------------------------|--------------------------------------------------------------------------|
| <b>Methods of Content Interaction</b> | Lecture, Tutorials, Group discussion; self-study, seminar, presentations |
|---------------------------------------|--------------------------------------------------------------------------|

### Course Objectives

- To impart knowledge about the advanced materials and its characteristics
- To equip the students with skills in materials synthesis
- To make students aware of emerging materials and conducting polymers
- To acquaint the students with the salient features of nanomaterials
- To make students learn about the structure and properties of intercalation compounds, composites and amorphous materials

### Learning Outcomes

After completion of the course the learners will be able to:

- Explain the relevance of advanced materials in daily life
- Distinguish between different type of materials based on structure and properties.
- Synthesize materials using different methods such as sol-gel, spray pyrolysis, combustion, hydrothermal, electrosynthesis etc.
- Analyze properties of different types of materials such as nanomaterials, intercalation compounds, perovskites etc.

## UNIT-I

**Classification of materials:** level of structures, Principles of self-assembly: surfactant solutions, importance of non-covalent forces, the hydrophobic effect, cooperativity, statistical mechanics of one-dimensional self-assembly.

**Principles and parameters** of solid-state synthesis, Fundamentals of sol-gel, precipitation, hydrolysis, combustion, microwave, carbothermal and mechano synthesis. Low temperature and gas phase synthesis techniques. Molten salt synthesis. Spray pyrolysis, chemical vapour deposition and sputtering techniques.

Intercalation and deintercalation. Intercalation reactions layered structure-graphite interlayer compounds (GILC), staging of graphite, TaS<sub>2</sub>.

## UNIT-II

**Nanomaterials:** Classification, synthesis, characterization and applications of nanoparticles, nano wires and nanotubes. Elemental nanoparticles: Pure, Gold, Silicon, Silver, Cobalt, Oxide nanoparticles: Silica, Zinc oxide, Iron oxide, Alumina. Stabilization of colloidal nanoparticles.

**Semiconductor nanoparticles:** Quantum confinement effects, size dependent optical properties; Magnetic nanoparticles: superparamagnetism, SPIONs, Giant magnetoresistance (GMR). Carbon based nanomaterials: carbon nanotubes, graphenes, and carbon dots. Nano Composites.

## UNIT-III

**Fullerenes and fullerides**– structure, synthesis, functionalization approaches, conducting properties of fullerides and applications.

High-Tc Oxides-structure, perovskite A & B, structure and synthesis of La, Sr and Ba cuprates, applications.

Conducting polymers - PA, PPP, PPS, PPY-mechanism of conduction and applications.

Microporous materials – zeolites and zeolitic materials,  $\text{AlPO}_4$ - $\text{GaPO}_4$ .

**Fibres and Composites:** Synthetic inorganic polymers- zirconia and other fibre Classification, microscopic composites, dispersion strengthened, particle reinforced, Fibre-glass reinforced composites, metal-matrix, plastic matrix composites, hybrid composites.

#### UNIT-IV

**Amorphous Materials:** Crystalline versus amorphous solids, glass formation, Preparation techniques melt spinning, sputtering, ion implantation, and Structural models of amorphous materials, Properties of met glasses-mechanical, electronic and magnetic properties.

**Liquid Crystals:** Mesomorphic behaviour, classification, examples - thermotropic and lyotropic liquid crystals Calamitic, nematic phase A, B, smectic phase, chiral nematic phase and optical Properties of liquid crystals.

**Superconducting Materials:** Transition Temperature, Meissner– Ochsenfeld Effect, Type I Superconductors, Type II Superconductors synthesis and structure of high temperature super conductors; Oxyhalides, oxycarbonates, boro carbides, cuprates materials and related preparation methods, making of films of superconductor.

**3-D Printing of materials and devices:** Fundamentals of 3D printing (additive manufacturing), Implications of 3D printing in chemicals and biological sciences, PDMS based microfluidic devices, 3D printing of Li-ion battery, hydrogels, bone replicate materials, calcium phosphate ceramics.

#### SUGGESTED BOOKS

1. Electrochemical Methods- Fundamentals and Applications, 2<sup>nd</sup> Edn, by A J Bard and L R Faulkner, John Wiley & Sons Inc., New York (2001).
2. Modern Electrochemistry, Vol.1, 2A and 2B by Bockris and Reddy, Plenum, N.Y (2000).
3. Magnetochemistry, R.L. Carlin, Springer Verlag.
4. Dana, M. Spence, Evaluation of 3D Printing and Its Potential Impact on Biotechnology and the Chemical Sciences, Analytical Chemistry, (ACS)
5. Nanostructured Materials: Processing, Properties and Applications, ed. C. C. Koch, Willaim Andrew Publishing, New York, 2002.
6. Nanomaterials: Synthesis, properties and applications, Ed. By A. S. Edelstein and R.C. Cammarata, Inst. of Physics, UK 1966.
7. Science of Engineering Materials, C.M. Srivastava and C. Srinivasan, Wiley-Eastern Ltd. (1991).
8. Solid State Chemistry and its Applications, A.R. West, John Wiley & Sons.(1989).
9. Material Science and Engineering. W.D. Callister, John Wiley and Sons Inc. (1985).
10. Nanotubes and Nano wires CNR Rao, & A Govindaraj, RSC, London 2005.
11. NANO: The essentials T. Pradeep, McGraw-Hill, 2008.

12. Liquid Crystals, Nature's delicate phase of matter, Peter J Collings, Princeton University Press, 2002.
13. Nanochemistry, A chemical approach to Nanomaterials, Geoffrey A Ozin and Andre C Arsenault, RSC, 2006.

| <b>Course Title: Advanced Quantum Mechanics and Surface Chemistry</b> |                                                                          |                        |                          |
|-----------------------------------------------------------------------|--------------------------------------------------------------------------|------------------------|--------------------------|
| <b>Course Code</b>                                                    | <b>CHE92DC03704</b>                                                      | <b>Credits</b>         | 4                        |
| <b>L + T + P</b>                                                      | 3 + 1 + 0                                                                | <b>Course Duration</b> | One Semester             |
| <b>Semester</b>                                                       | Even                                                                     | <b>Contact Hours</b>   | 45 (L) + 15 (T)<br>Hours |
| <b>Methods of Content Interaction</b>                                 | Lecture, Tutorials, Group discussion; self-study, seminar, presentations |                        |                          |

### Course Objectives

Students proficient in various methods such as Heitler-London method, HF-SCF-LCAO To acquaint students with advanced level concepts in quantum mechanics

- To make students aware of various advanced level concepts in surface chemistry such as Hertz-Knudsen equation, Langmuir-Rideal mechanism, Rideal-Eley mechanism etc.
- To make students learn methods to determine surface structure such as Harkins-Jura method, radioactive tracer method and Benton and White method
- To impart knowledge about instrumental techniques such as SEM, TEM. STM and AES for surface analysis

**Learning Outcomes:** After completion of the course the learners will be able to:

- Apply the concept and write quantum mechanical equations for simple molecules such as  $H_2$ ,  $H_2^+$  etc.
- Write expressions in terms of wave functions for hybrid orbitals, localized and delocalized molecular orbitals in polyatomic molecules
- Determine the rate and entropy of adsorption
- Determine the surface structure using different instrumental techniques.

### UNIT-I

**Quantum Chemistry-I: Theories of valence:** Introductory aspects: Linear and non-linear variation functions. Secular equations. Coulombic, exchange, normalization and overlap integrals. Secular determinants. Molecular orbital (MO) theory, LCAO-MO approximation, application to Hydrogen molecule ion ( $H_2^+$ ), energy levels of  $H_2^+$ , bonding and antibonding molecular orbitals, electron distribution, potential energy diagrams, comparison of theoretical and experimental values of energy. Valence bond (VB) theory of  $H_2$  molecule, the Heitler-London method, energy levels, energy distribution. Various modifications of the Heitler-London wave function.

Comparison of MO and VB theories. Ionic terms, fractional ionic characters and its importance, Equivalence of simple MO and VB methods ion-covalent resonance and configuration interaction. LCAO treatment of diatomic molecules, LCAO forms of simple

wave function and molecular orbitals. Notations of molecular orbitals: full notation, Mulliken notation. MO configuration of homo- and hetero- nuclear diatomic molecules. Molecular electric terms. Bond order, stability and magnetic behaviour of molecules from M.O. diagrams, isoelectronic systems. Correlation diagrams, non-crossing rule.

## UNIT-II

**Quantum Chemistry-II:** The HF-SCF-LCAO method. Directed valence, hybridization, Expressions for hybrid orbitals in terms of wave functions of s and p orbitals and explanation of directed valences of  $sp$ ,  $sp^2$ , and  $sp^3$  hybrid orbitals. Hybridization involving d-orbitals, Localized and non-localized molecular orbitals in polyatomic molecules ( $H_2O$ ).

Huckel molecular orbital theory: Outline of the method including assumptions. Application to ethylene, allyl radical, cyclo-propenyl radical, butadiene, cyclobutadiene, bicyclo-butadiene and benzene. Calculation of delocalization energy, charge density,  $\pi$ -mobile bond order and free valence.

## UNIT-III

### SURFACE CHEMISTRY-I

- A. Review of adsorption curves, Adsorption-desorption, Adsorption forces, Heat of adsorption-Types, Measurements of heat of adsorption (Calorimetric and Clausius Clapeyron method), Measurement of adsorption isotherms, (Volumetric and Gravimetric methods), Determination of entropy of adsorption,
- B. Electrostatic adsorption, adsorption indicators and their applications. Volcanic curves. Applications of adsorption.
- C. Adsorption kinetics: Kinetics of chemisorption (Hertz-Knudsen equation), Chemisorptive bond, Competitive adsorption, Mechanism of some catalyzed surface reactions, Kinetic effects of surface heterogeneity, Kinetic effects of interactions, Potential energy curves for adsorption, Transition state theory of surface reactions, Rates of desorption, Kinetics of bimolecular surface reactions, Langmuir-Hinshelwood Mechanism, Langmuir-Rideal mechanism, Rideal-Eley mechanism and their comparison.
- D. Adsorption theories: Polanyi's potential theory and Polarization theory. Hysteresis of adsorption.

## UNIT-IV

### SURFACE CHEMISTRY-II

Surface structure: Surface mobility, Surface heterogeneity, Surface and its determination by point-B method, Harkins-Jura method, radioactive tracer method and Benton and White method. Importance of surface area. Examination of surfaces by Interferometer method, Scanning electron microscopy (SEM), Low energy electron diffraction method (LEED method), Field Emission spectroscopy, Auger electron spectroscopy (AES), STM, and TEM.

### SUGGESTED TEXT BOOKS

1. Molecular Quantum mechanics, P.W. Atkins and R.S. Friedman, Oxford University press (1997).
2. Introductory Quantum Chemistry by A.K. Chandra, Tata McGraw Hill (1994).

- Quantum Chemistry by R.K. Prasad, 3<sup>rd</sup> Edn, New Age International (2006).
- Quantum Chemistry by Ira N. Levine, Prentice Hall, New Jersey (1991).
- Quantum Chemistry by Donald A McQuarrie, Viva Books Pvt. Ltd. New Delhi, India, Published in arrangement with University Science books, Sausalito, CA, USA (2003).
- Physical chemistry of surfaces by A. W. Adamson, Interscience Publishers Inc., New York (1967).
- Surface Chemistry: Theory and Applications by J.J. Bikertman, Academic Press, New York (1972).
- Chemical Kinetics by K.J. Laidler, 3<sup>rd</sup> Edn., Harper International Edn., (1987).
- Text Book of Physical Chemistry by S. Glasstone, McMillan India Ltd. 2<sup>nd</sup> Edn. (1986).
- Physical chemistry, R.J. Silbey, R.A. Alberty and M.G. Bawendi Edn, Wiley (2009).
- Physics at surfaces, A. Zangwill, Cambridge University Press (1988).
- Surface crystallography, L.J. Clarke, Wiley-Interscience (1985).

| <b>Course Title: Applications of spectroscopy techniques to inorganic systems</b> |                                                                          |                        |                          |
|-----------------------------------------------------------------------------------|--------------------------------------------------------------------------|------------------------|--------------------------|
| <b>Course Code</b>                                                                | <b>CHE92DC01604</b>                                                      | <b>Credits</b>         | 4                        |
| <b>L + T + P</b>                                                                  | 3 + 1 + 0                                                                | <b>Course Duration</b> | One Semester             |
| <b>Semester</b>                                                                   | Even                                                                     | <b>Contact Hours</b>   | 45 (L) + 15 (T)<br>Hours |
| <b>Methods of Content Interaction</b>                                             | Lecture, Tutorials, Group discussion; self-study, seminar, presentations |                        |                          |

#### **Course Objectives**

- To enhance the understanding of vibrational spectroscopy and discuss some specific cases of ambidentate, multidentate ligands and multinuclear complexes
- To lay the foundations of Raman spectroscopy
- To acquaint the students with the core concepts of photoelectron spectroscopy and NMR spectroscopy and discuss its application in inorganic chemistry
- To highlight the efficacy of ESR (Electron Spin Resonance) spectroscopy in elucidating the structure and properties of inorganic complexes and free radicals.
- To acquaint the students with these less common techniques such as Mossbauer spectroscopy, NQR and X-ray absorption spectroscopy

**Learning Outcomes:** After completion of the course the learners will be able to:

- Analyze the FTIR spectra of mononuclear and multinuclear metal complexes with multidentate and ambidentate ligands
- Apply Raman spectroscopy to elucidate the structure and bonding of inorganic systems including the IR inactive ones
- Use NMR and photoelectron spectroscopy to explain structure and bonding in inorganic compounds

- Determine the structure and bonding in paramagnetic complexes and free radicals using ESR spectroscopy
- Apply Mossbauer spectroscopy technique to explain the magnetic properties of iron and tin-based compounds

### UNIT-I

**Vibrational spectroscopy (IR and Raman):** Vibrational spectra of diatomic, linear and bent triatomic, AB<sub>3</sub>, AB<sub>4</sub>, AB<sub>5</sub> and AB<sub>6</sub> molecules, spectra of metal complexes: Ammine, amido, Nitro, Nitrito, lattice water, aquo and hydroxo, carbonato, nitrato, sulphato and other acido complexes, cyano and nitrile complexes, cyanato and thiocyanato complexes, mono and multinuclear carbonyl complexes, nitrosyls, phosphines and arsines, ambidentate ligands, ethylenediamine and diketonato complexes. Structural determination using Raman and IR spectroscopy, symmetry of metal- complexes and IR spectra. Understanding hydrogen bonding through IR and Raman spectroscopy.

### UNIT-II

**Photoelectron spectroscopy:** Basic principles- photoelectric effect, Koopman's theorem, XPS and UPS, spin-orbit coupling in core level spectra, applications of core level spectra- ESCA, chemical shift, Valence level spectra- n, and bands, Auger electron spectroscopy and applications, Electron energy loss spectroscopy- basic principles and applications to the study of solids

**Mass spectrometry:** Basic principles and instrumentation, mass spectral fragmentation of inorganic compounds, applications to organometallic compounds. Effect of isotopes on the appearance of a mass spectrum, molecular weight determination, thermodynamic data.

### UNIT-III

**NMR spectroscopy of inorganic molecules:** Proton NMR spectra of metal hydride complexes NMR spectra of nuclei other than hydrogen: <sup>19</sup>F, <sup>31</sup>P, <sup>11</sup>B NMR spectra of simple compounds, Proton / hydride interactions with <sup>103</sup>Rh, <sup>183</sup>W, <sup>195</sup>Pt and <sup>207</sup>Pb in metal complexes / organometallic compounds, Solid State NMR, Berry Pseudo rotation and NMR spectra, variable temperature NMR spectra.

**Electron spin resonance spectroscopy:** Basic principles, the position of ESR absorption, significance of 'g' factor, determination of 'g' factor. Electron- nucleus coupling (Hyperfine splitting). ESR spectrometer, electron- electron coupling, Interpretation of ESR spectra and structure elucidation of organic radicals using ESR spectroscopy. Spin density and McConnell relationship. Spin polarization for atoms and transition metal ions, spin-orbit coupling and significance of g-tensors, zero/non-zero fieldsplitting, Kramer's degeneracy, application to transition metal complexes (having one to five unpaired electrons) including biological molecules and inorganic free radicals such as PH<sub>4</sub>, F<sub>2</sub> and BH<sub>3</sub>.

### UNIT-IV

**Mossbauer spectroscopy:** Basic principles, isomershift, quadrupole splitting and magnetic hyperfine interactions, application to the study of bonding and structures of Fe<sup>2+</sup> and Fe<sup>3+</sup> compounds, Sn<sup>2+</sup> and Sn<sup>4+</sup> compounds.

**NQR spectroscopy:** NQR isotopes, electric field gradients, Nuclear Quadrupole coupling constants, Experimental techniques and applications

**X-ray absorption spectroscopy:** Near edge measurements and EXAFS.

### SUGGESTED BOOKS

1. Physical methods in Inorganic Chemistry, R.S.Drago, Affiliated East West Press Pvt. Ltd., New Delhi (1965).
2. Infrared spectra of Inorganic and Coordination Compounds, K.Nakamoto, Wiley Interscience, New York (1970).
3. Vibrational Spectroscopy: Theory and Applications, D.N.Sathyanarayana, New Age International Publishers, New Delhi (2000).
4. Electronic Absorption Spectroscopy and Related Techniques, D.N. Sathyanarayana, Universities Press, Bangalore (2001).

| Course Title: Spectroscopy and Chiroptical properties |                                                                          |                 |                       |
|-------------------------------------------------------|--------------------------------------------------------------------------|-----------------|-----------------------|
| Course Code                                           | CHE92DC02604                                                             | Credits         | 4                     |
| L + T + P                                             | 3+1+0                                                                    | Course Duration | One Semester          |
| Semester                                              | Even                                                                     | Contact Hours   | 45 (L) + 15 (T) Hours |
| Methods of Content Interaction                        | Lecture, Tutorials, Group discussion; self-study, seminar, presentations |                 |                       |

**OBJECTIVE:** To develop an understanding of the basic principles of spectroscopy and to learn to apply these principles for structural elucidation of simple organic compounds. To build up a knowledge about the basic principle of catalysis in organic reactions.

### UNIT I

**UV spectroscopy:** Introduction, absorption laws, instrumentation, formation of absorption bands, types of electronic transitions, chromophores, auxochromes, absorption and intensity shifts, solvent effects, Woodward-Fieser rules for calculating absorption maximum in dienes and  $\alpha,\beta$ -unsaturated carbonyl compounds.

**IR spectroscopy:** Introduction, theory of molecular vibrations, vibrational frequency, factors influencing vibrational frequencies, finger print region and applications of IR spectroscopy.

### UNIT II

**Structure elucidation by NMR spectroscopy:** Introduction, Magnetic properties of nuclei-Resonance condition, Nuclear spin, population of nuclear spin levels and NMR isotopes, Relaxation methods, Instrumentation; Classical approach.

Chemical shift, Factors influencing chemical shifts: electronegativity and electrostatic effects; Mechanism of shielding and deshielding in alkanes, alkyl halides, alkenes, aromatic compounds, carbonyl compounds and annulenes. Pascal triangle-low and high resolution, Reference compounds (internal and external reference compounds) Karplus Curve, Diamagnetic and Paramagnetic effects and Magnetic anisotropy. Equivalence of protons-chemical and magnetic equivalence; Spin systems: First order and second order coupling of AB systems, Simplification of complex spectra.



**Spin-spin interactions:** Homonuclear coupling interactions-AX, AX<sub>2</sub>, AX<sub>3</sub>, AMX, AB types. Vicinal, germinal and long-range coupling-spin decoupling; Chemical shift reagents and deuterium exchange; stereochemistry and hindered rotations. Temperature effects.

<sup>1</sup>H-NMR spectrums of F and P containing organic molecules.

CIDNP, Nuclear Overhauser effect (NOE), Factors influencing coupling constants and Relative intensities.

Two- dimensional NMR spectroscopy, COSY, NOESY, HMBC, HMQC, DEPT and INEPT, DOESY terminologies.

**<sup>13</sup>C NMR Spectroscopy:** Types of CMR spectra-undecoupled, proton decoupled, off-resonance decoupled (SFORD); Selectively decoupled and gated decoupled spectra. <sup>13</sup>C-chemical shifts of alkanes, alkyl halides, alkenes, alkynes, alcohols, ethers, carbonyl compounds and aromatic compounds; Factors affecting the chemical shifts. Applications of <sup>13</sup>C-NMR spectroscopy in confirmation of structure and stereochemistry of organic molecules and in determining the reaction mechanism and dynamic processes of organic reactions—example

Applications of NMR in organic chemistry as elucidation of the structure of unknown compounds.

### UNIT III

**Mass Spectrometry:** Introduction, ion production—EI, CI, FD and FAB, factors affecting fragmentation, ion analysis, and ion abundance. Mass spectral fragmentation of organic compounds, common functional groups, Molecular ion peak, Meta-stable peak, McLafferty rearrangement. Nitrogen Rule. High-resolution mass spectrometry. Examples of mass spectral fragmentation of organic compounds with respect to their structure determination. Introduction to negative ion Mass spectrometry, TOF-MALDI. Problems based upon IR, UV, NMR and mass spectroscopy.

### UNIT IV

**Molecular dissymmetry and chiroptical properties:** Linear and circularly polarised lights, circular birefringence and circular dichroism, ORD and CD curves, Cotton effect. The axial halo ketone rule, octant diagrams, helicity, and Lowe's rule. Application of ORD and CD to structural and stereochemical problems.

### SUGGESTED TEXT BOOKS

1. Kemp, W. Organic Spectroscopy 3<sup>rd</sup> Ed., W. H. Freeman & Co. (1991).
2. Silverstein, R. M., Bassler, G. C. & Morrill, T. C. *Spectroscopic Identification of Organic Compounds* John Wiley & Sons (1981).
3. NMR Spectroscopy, H. Gunther, 2<sup>nd</sup> ed.; John Wiley and Sons, 1995.
4. ORD and CD in Chemistry and Biochemistry, 1972, PIERRE CRABBÉ.

### SUGGESTED REFERENCE BOOKS

1. Electron Paramagnetic Resonance of Transition Metal ions, A. Abragam, B. Bleaney, Oxford University Press, 1970.
2. Physical Methods for Chemist, R. S. Drago, Saunders, 1992.

3. Fundamentals of Molecular Spectroscopy, C. N. Banwell and E. M. McCash, 4<sup>th</sup> ed, McGraw-Hill, 1994.
4. Spectroscopic methods in organic chemistry, D. H. Williams, I. Fleming, Tata McGraw Hill. 1988.
5. Symmetry, Spectroscopy, and Crystallography: The Structural Nexus, Robert Glaser, Wiley, 2015.

|                                          |                                                                          |                        |                       |
|------------------------------------------|--------------------------------------------------------------------------|------------------------|-----------------------|
| <b>Course Title: Lasers in Chemistry</b> |                                                                          |                        |                       |
| <b>Course Code</b>                       | <b>CHE92DC03804</b>                                                      | <b>Credits</b>         | 4                     |
| <b>L + T + P</b>                         | 3 + 1 + 0                                                                | <b>Course Duration</b> | One Semester          |
| <b>Semester</b>                          | Even                                                                     | <b>Contact Hours</b>   | 45 (L) + 15 (T) Hours |
| <b>Methods of Content Interaction</b>    | Lecture, Tutorials, Group discussion; self-study, seminar, presentations |                        |                       |

### Course Objectives

To acquaint the students with the fundamentals of lasers and its use in chemistry

- To make students aware of different types of laser sources such as, solid state lasers, He-Ne Lasers, Exciplex lasers etc,
- To make students learn how lasers are integrated and used in some well-known analytical techniques such as chromatography, polarimetry etc.
- To make students learn the application of lasers in driving photochemical reactions and in inducing therapeutic effects such as photodynamic and photothermal therapy
- To develop an understanding of laser-based spectroscopy techniques such as Laser Stark Spectroscopy, Absorption Spectroscopy, Laser Magnetic Resonance, Fluorescence Spectroscopy etc.

### Learning Outcomes

After completion of the course the learners will be able to:

- Distinguish between coherent and non-coherent light sources
- Explain the basic concepts involved in making and working of lasers
- Discuss the salient features of various lasers such as semiconductor lasers, exciplex lasers, solid state, molecular gas lasers etc
- Explain how advent of lasers have enhanced the efficacy of various analytical techniques such as chromatography, polarimetry etc.
- Examine and evaluate the relevance of lasers in daily life such as its use in photochemical reactions and photodynamic/photothermal therapy
- Underscore the importance of laser-based spectroscopic techniques

## UNIT I

### Operation of Laser

The Nature of Stimulated Emission, Resonators and Pumping Processes, Coherent Radiation, Standing Waves and Modes, The Kinetics of Laser Emission: Rate Equations,

Threshold Conditions, Pulsed Versus Continuous Emission; Transitions, Lifetimes and Line widths: Three-level Laser, Four-level Laser, Emission Line widths; Properties of Laser Light, and Their Applications: Beam width, Coherence, Intensity, Monochromaticity

## **UNIT II**

### **Laser Sources**

Solid-state Transition Metal Ion Lasers: Ruby Laser, Neodymium Lasers; Semiconductor Lasers, Atomic and Ionic Gas Lasers: Helium-neon Laser, Argon Laser, Copper Vapour Laser; Molecular Gas Lasers: Carbon Dioxide Laser, Nitrogen Laser, Chemical Lasers, Iodine Laser, Exciplex Lasers; Dye Lasers, Free-electron Lasers

### **Laser Instrumentation in Chemistry**

Polarising Optics, Frequency Conversion, Pulsing Techniques: Cavity Dumping, Q-Switching, Mode-locking; Detectors, Pulse Detection Systems: Lock-in Amplifiers, Boxcar Integrators, Single-pulse Systems; Light Scattering Instrumentation: Nephelometry, Photon Correlation Measurements, Brillouin Scattering, Doppler Velocimetry, Lidar; Polarimetry, Laser Detectors in Chromatography, Laser Microprobe Instrumentation

## **UNIT III**

### **Laser-Induced Chemistry**

Principles of Laser-induced Chemistry: Multiphoton Infra-red Excitation, Reaction Rates and Yields; Laser Photochemical Processes: Unimolecular Laser-induced Reactions, Bimolecular Laser-enhanced Reactions, Laser-sensitised Reactions, Laser Surface Chemistry, Ultrafast Reactions, Laser Reaction Diagnostics; Isotope Separation: Photo ionisation, Photo dissociation, Photochemical Reaction, Photo deflection; Miscellaneous Applications: Purification of Materials, Production of Ceramic Powders, Photodynamic and Photothermal therapy.

## **UNIT IV**

### **Spectroscopy with Lasers**

Absorption Spectroscopy, Specialised Absorption Techniques: Excitation Spectroscopy, Ionisation Spectroscopy, Thermal Lensing Spectroscopy, Photo acoustic Spectroscopy, Optogalvanic Spectroscopy, Laser Magnetic Resonance,

Laser Stark Spectroscopy; Fluorescence Spectroscopy: Laser-induced Atomic Fluorescence, Laser-induced Molecular Fluorescence; Raman Spectroscopy

## **SUGGESTED TEXT BOOKS**

1. D. L. Andrews, Lasers in Chemistry, Springer, Heidelberg
2. S. Chopra, Lasers in Chemical and Biological Sciences, New Age International Publishers (1992).
3. H. H. Telle, A. G. Ureña, R. J. Donovan, Laser Chemistry: Spectroscopy, Dynamics and Applications, Wiley publications (2007)
4. M. Lackner, Lasers in Chemistry, Vol. I & Vol. II., Wiley VCH (2008).

## ELECTIVES COURSES

### For DE/OE

| Course Title: Basics of Supramolecules and its advancement |                                                                          |                 |                          |
|------------------------------------------------------------|--------------------------------------------------------------------------|-----------------|--------------------------|
| Course Code                                                | DE01004/ OE01004                                                         | Credits         | 4                        |
| L + T + P                                                  | 3 + 1 + 0                                                                | Course Duration | One Semester             |
| Semester                                                   | Odd                                                                      | Contact Hours   | 45 (L) + 15 (T)<br>Hours |
| Methods of Content Interaction                             | Lecture, Tutorials, Group discussion; self-study, seminar, presentations |                 |                          |

#### Course Objectives

- To acquaint students with the fundamentals of supramolecule and macromolecule
- To impart knowledge and skills for the synthesis of supramolecular structures
- To introduce the concept of self-assembly and its mechanistic aspects
- To make students aware of device applications of supramolecular structures

**Learning Outcomes:** After completion of the course the learners will be able to:

- Explain the binding interactions in supramolecular structures
- Write the synthesis scheme and structures of crown ethers, host-guest compounds
- Apply the concept of 'self-assembly' to make supramolecular structures
- Discuss the relevance of supramolecular structures in daily life and its applications in molecular devices, medicine, and catalysis.

#### UNIT I

##### Supramolecular interactions

Definition of supramolecular interaction. Nature of binding interactions in supramolecular structures: ion-ion, Ion-dipole, dipole-dipole, H-bonding, cation-p, anion-p, p-p, and van der Waals interactions. Host Guest interactions, preorganization and complementarity, lock, and key analogy. Binding of cationic, anionic, ion pair and neutral guest molecules. The role of solvents in supramolecular systems.

#### UNIT II

##### Synthesis and Structure of Supramolecules

Self-assembly molecules: design, synthesis and properties of the molecules, self-assembling by H-bonding, metal-ligand interactions, and other weak interactions, metallomacrocycles, catenanes, rotaxanes, helicates and knots. Synthesis and structure of crown ethers, lariat ethers, podands, cryptands, spherands, calixarenes, cyclodextrins, cyclophanes, cryptophanes, carcerands and hemicarcerands.

#### UNIT III

##### Applications of Supramolecules

**Molecular devices:** molecular electronic devices, molecular wires, molecular rectifiers, molecular switches, molecular logic, molecular tweezers. Supramolecules as mimic for biological systems: cyclodextrins as enzyme mimics, ion channel mimics, supramolecular catalysis etc. Supramolecular gel and polymerization.

## UNIT IV

### Recent advancement in supramolecular chemistry

**Supramolecular system chemistry:** equilibrium assemblies, kinetically trapped assemblies, far-from equilibrium assemblies, dissipative non-equilibrium self-assembly, supramolecular metal organic framework.

**Supramolecular adaptive chemistry:** molecular information, recognition, and receptors. Criteria for the selection of self-organization, supramolecular dynamic non-covalent interactions, supramolecular dynamics, constitutional dynamic synthesis of supramolecules.

### SUGGESTED TEXT BOOKS

1. Supramolecular Chemistry- Concepts and Perspectives (Wiley-VCH, 1995), J.-M. Lehn.
2. Bioorganic, Bioinorganic and Supramolecular Chemistry, P. S. Kalsi and J. P. Kalsi. New Age International Publishers.

### SUGGESTED REFERENCE BOOKS

1. P. D. Beer, P. A. Gale, D. K. Smith; Supramolecular Chemistry (Oxford University Press, 1999).
2. J. W. Steed and J. L. Atwood; Supramolecular Chemistry (Wiley, 2000).

| Course Title: Green Chemistry I: Solvents & Synthesis |                                                                          |                 |                       |
|-------------------------------------------------------|--------------------------------------------------------------------------|-----------------|-----------------------|
| Course Code                                           | DE02004 / OE02004                                                        | Credits         | 4                     |
| L + T + P                                             | 3 + 1 + 0                                                                | Course Duration | One Semester          |
| Semester                                              | Odd                                                                      | Contact Hours   | 45 (L) + 15 (T) Hours |
| Methods of Content Interaction                        | Lecture, Tutorials, Group discussion; self-study, seminar, presentations |                 |                       |

### Course Objectives

- To make students understand the principles and goals of green chemistry
- To acquaint with the concept of green solvents and to understand the need for alternative solvents
- To develop an understanding of supercritical fluids, biphasic systems and ionic liquids
- To equip the students with necessary skills to do radiation-based synthesis

**Learning Outcomes:** After completion of the course the learners will be able to:

- Distinguish between a green-process and non-green process
- Design alternative routes of synthesis which is greener, cleaner and cost-effective
- Perform radiation-based synthesis such as sonochemical and microwave
- Conduct solvent-less synthesis

## UNIT-I

**Introduction:** Need for Green chemistry – Goals of green chemistry; principles of green chemistry with their explanations and examples – Designing a green synthesis – Prevention of

waste / by products – Atom economy (maximum incorporation of materials used in the process) – Minimization of hazardous / toxic products – prevention of chemical accidents

## UNIT-II

**Green Solvents:** Role of solvents in chemical synthesis, Environmental and health concerns of organic solvents, Need for Alternative/Cleaner solvents, Criteria for selection and design of green solvents

**Water:** The natural solvent on earth, organic reactions: hydrophobic effects enhancing the reaction selectivities, low solubility of O<sub>2</sub> in water, water soluble catalysts, challenges in using water as solvent,

**Ionic liquids:** physicochemical properties, Synthesis of Ionic Liquids, Directed Inorganic and Organometallic Synthesis, formation of oxides, electrochemical synthesis in ionic liquids,

**Glycerol:** solvent properties, volatility, polarity, availability, glycerol as a solvent combining the advantages of water and ionic liquids, enhancement of reaction selectivity, glycerol as a solvent for catalyst design and recycling, separation processes and material synthesis in glycerol, examples of synthesis of transition metal and metal oxide crystals

**Supercritical fluids:** supercritical CO<sub>2</sub> and its properties, advantages of using CO<sub>2</sub> as solvent, Synthesis of metal nanoparticles, CO<sub>2</sub> as solvent for coatings and lithography, biomaterial processing, other supercritical fluids.

**Biphasic systems:** Liquid-liquid interface, aqueous biphasic systems, phase- and micelle forming polymers for clean separation processes, Fluorous biphasic catalysis (FBC)

## UNIT-III

### Radiation based techniques in green synthesis

**Microwave:** microwave as a form of electromagnetic radiation, interaction of materials with microwaves and dielectric heating, microwave reactors, Different types of reactions involved in microwave synthesis (i) direct reactions, including those involving the use of simple compounds; Hoffmann Elimination, Diels Alder reaction, (ii) preparation of solids which involve decompositions and combinations giving rise to solids of complex composition; (iii) nitridation reactions; (iv) reactions brought about in liquid media; (v) preparation of glasses; (vi) selective deoxidation reactions; and (vii) plasma-assisted reactions. Microwave synthesis of zeolite membranes & other examples.

## UNIT IV

**Sonochemical:** ultrasound waves, basic principles of sonochemistry, acoustic cavitation phenomenon, Stable and transient cavitation, Temperatures of cavitation, Cold sono-fusion, Hydrodynamic cavitation, From cavitation to chemistry, generation of free radicals, sonochemical reactions, sono-oxidation, sono-reduction, sonication in ionic liquids, ultrasound and photochemistry, Combined use of ultrasound and microwaves, some examples of sonochemical synthesis. Esterification, Saponification

## SUGGESTED TEXT BOOKS

1. Ionic Liquids in Synthesis, Peter Wasserscheid and Tom Welton, WILEY-VCH Verlag GmbH & Co. KGaA, 2008.

2. Green Chemistry and Catalysis, R.A. Sheldon, I. Arends and U. Hanefeld, WILEY-VCH Verlag GmbH & Co. KGaA (2007).
3. Green Solvents for Chemistry: Perspectives and Practice, William M. Nelson Oxford University Press (2003).
4. Biocatalysis for Green Chemistry and Chemical Process Development, Junhua Tao and Romas Joseph Kazlauskas, WILEY-VCH Verlag GmbH & Co. KGaA (2011).
5. Green chemistry for chemical synthesis, Chao-Jun Li and Barry M. Trost, Proceedings of National Academy of Sciences (USA), year 2008, vol. 105, pages 13197–13202.
6. Advances in inorganic chemistry, Elsevier, Vol. 58, (2006).
7. Green Catalysis, Masaya Matsuoka and Masakazu Anpo, Wiley-VCH Verlag GmbH & Co. KGaA (2010).
8. A primer on electrocatalysis, J.O'M. BOCKRIS, J. Serb. Chem. Soc. 70 (3) 475–487 (2005).
9. Direct Electrochemistry of Hemoglobin and Its Electrocatalysis Based on Hyaluronic Acid and Room Temperature Ionic Liquid, Electroanalysis 20, 2008, No. 23, 2537 – 2542.
10. Photocatalysis. A multi-faceted concept for green chemistry, D.Ravelli, D. Dondi, M. Fagnonia and A. Albini, Chem. Soc. Rev., 2009, 38, 1999–2011.
11. Synthesis of Inorganic Solids Using Microwaves, K. J. Rao, B. Vaidhyanathan, M. Ganguli, and P. A. Ramakrishnan, Chemistry of Materials, 1999, 11, 882-895.
12. Sonochemistry and sonoprocessing: the link, the trends and (probably) the future, Timothy J. Mason, Ultrasonics Sonochemistry 10 (2003) 175–179.

| <b>Course Title: Solid State and Structural Chemistry</b> |                                                                          |                        |                       |
|-----------------------------------------------------------|--------------------------------------------------------------------------|------------------------|-----------------------|
| <b>Course Code</b>                                        | <b>DE03004 / OE03004</b>                                                 | <b>Credits</b>         | 4                     |
| <b>L + T + P</b>                                          | 3 + 1 + 0                                                                | <b>Course Duration</b> | One Semester          |
| <b>Semester</b>                                           | Even                                                                     | <b>Contact Hours</b>   | 45 (L) + 15 (T) Hours |
| <b>Methods of Content Interaction</b>                     | Lecture, Tutorials, Group discussion; self-study, seminar, presentations |                        |                       |

#### **Course Objectives**

- To acquaint the students with the electronic and magnetic properties of the solids
- To introduce the emerging concepts of piezoelectricity, ferroelectricity and dielectrics
- To equip the students with necessary skills in geometrical crystallography
- To make students learn the concepts and techniques of structure determination [x-ray diffraction (XRD), neutron diffraction (ND), electron diffraction (ED)]

**Learning Outcomes:** After completion of the course the learners will be able to:

- Identify the symmetry elements in a solid and assign a point group

- Explain the band structure of solids
- Understand and apply concepts of piezoelectricity, ferroelectricity in daily life
- Determine the crystal structure using XRD & ED

### UNIT-I

**Electronic structure of solids:** Bonding in solids: Ionic, covalent, metallic and molecular solids free electron theory, Fermi sphere, Fermi-Dirac statistics, Ohm's law, limitations of the free electron theory.

Electrons in a weak periodic potential (Independent electron model), energy levels in extended, repeat and reduced zone schemes

**Electrical and Magnetic Properties of Solids Metals:** calculation of density of states, origin of resistivity, weak paramagnetism Semiconductors: Intrinsic and extrinsic- p and n-types, Hall Effect, Junctions and their applications- metal-metal, metal-semiconductor, semiconductor-semiconductor types and transistors.

**Insulators-** dielectric properties, piezo and inverse piezoelectric effects, ferroelectricity, ferroelectric transitions in  $\text{BaTiO}_3$ , ionic conductivity applications of band theory to TiO and NiO: Limitations of the Independent electron model, modelling electron correlation.

### UNIT-II

#### Geometric Crystallography

Symmetry elements, Bravais lattices, Screwaxes and glide planes, point groups, and space groups and nomenclature. Law of Interfacial angle (Euler's construction).

#### Diffraction theory and Single crystal X-ray diffraction

X-rays, Bragg's law, assignment of diffraction peaks, diffraction pattern of a primitive cubic lattice, space group extinctions, Scattering factor and structure factor, intensities from atomic positions for BCC and FCC lattices; Ewald's sphere of reflection, Reciprocal Lattice concept, Electron density function, Fourier synthesis, Fourier transform of the structure factor, Phase problem and Patterson synthesis.

### UNIT-III

**Experimental Methods:** Rotation, Oscillation, Weissenberg and Precession methods. Debye-Scherrer method (Powder method), Determination of lattice parameters from these methods.

### UNIT-IV

**Electron diffraction:** Experimental technique, Wierl equation, Radial-Distribution method.

**Neutron diffraction:** Principle and Theory, advantages and uses.

### SUGGESTED TEXT BOOKS

1. Introduction to Solids, L.V. Azaroff, McGraw Hill Book Co., New York, 1960.
2. Solid State Physics, N.W. Ashcroft and N.D. Mermin, Holt Saunders International Ltd., New York (1976).
3. Physical Chemistry, G.M. Barrow, McGrawHill (2<sup>nd</sup> ISE) (1966).
4. An Introduction to X-ray Crystallography, M. M. Woolfson, Cambridge University Press-Vikas Publishing House, New Delhi (1980).



5. Principles of the Solid State, H. V. Kheer, Wiley Eastern Ltd., New Delhi (1993).
6. Dynamics of Atoms in Crystals, W.Cochran, Edward Arnold, London,1973.(Pages24-37)
7. Vibrational Spectroscopy of Solids, P.M.A. Sherwood, University Press, Cambridge, 1972. (pages: 1-45)
8. Phase Transitions, C.N.R. Rao and K.J. Rao, Cambridge University Press
9. X-ray Structure determination : A practical guide, George H Stoutand Lyle H Jenson, Macmillan Publishing Co.Inc and Collier Macmillan Publishers

### SUGGESTED REFERENCE BOOKS

1. R. West, Solid State Chemistry and its Applications, John Wiley & Sons, 1984.
2. L. Smart and E. Moore, Solid State Chemistry - An Introduction, Chapman & Hall, 1992.
3. H. V. Keer, Principles of the Solid State, Wiley Eastern Limited, 1993.
4. K. Chakrabarty, Solid State Chemistry, New Age Publishers, 1996.

| <b>Course Title: Advanced Instrumental Techniques-I</b> |                                                                          |                        |                       |
|---------------------------------------------------------|--------------------------------------------------------------------------|------------------------|-----------------------|
| <b>Course Code</b>                                      | <b>DE03104 / OE03104</b>                                                 | <b>Credits</b>         | 4                     |
| <b>L + T + P</b>                                        | 3 + 1 + 0                                                                | <b>Course Duration</b> | One Semester          |
| <b>Semester</b>                                         | Odd                                                                      | <b>Contact Hours</b>   | 45 (L) + 15 (T) Hours |
| <b>Methods of Content Interaction</b>                   | Lecture, Tutorials, Group discussion; self-study, seminar, presentations |                        |                       |

### Course Objectives

- To equip the students with the knowledge and skills in advanced instrumental techniques
- To develop a comprehensive understanding of diffraction based techniques such as X-ray Diffraction (XRD), Electron Diffraction (ED) and Neutron Diffraction (ND)
- To make students learn the core concepts of absorption spectroscopic techniques such as UV-Vis absorption, FT-IR and Raman spectroscopy and its applications
- To impart knowledge and skills about the Resonance based techniques such as Mossbauer, NMR and EPR spectroscopy

### Learning Outcomes

After completion of the course the learners will be able to:

- Deduce the lattice structure by analyzing the XRD, ED and ND patterns
- Analyze the UV-Vis absorption, vibrational (FTIR, Raman) and rotational (microwave) spectra
- Apply Mossbauer spectroscopy technique to explain the hyperfine properties of iron and tin compounds

## UNIT I

### Diffraction based techniques

**Powder X-ray diffraction:** construction of the instrument, Identification of unknown materials, Determination of sample purity, Determination and refinement of lattice parameters, Determination of crystallite size/stress

**Single-crystal X-ray diffraction:** determination of crystal structure, position of H-atom in inorganic compounds, determination of bond lengths.

**X-ray diffraction using synchrotron source:** determination of complex molecules like proteins, enzymes. Neutron diffraction, electron diffraction

## UNIT II

### Absorption spectroscopy

**UV-Vis absorption :** construction of the instrument, measuring a spectrum, Beer-Lambert law, deviations from Beer's law, Relating UV-Vis spectra and colour, spectroscopic monitoring of titrations and kinetics

**FT-IR and Raman spectroscopy:** understanding the molecular vibrations and their energies, Complementary relationship between Raman and FTIR spectroscopy.

**FTIR spectroscopy:** construction of the instrument, dispersive and non-dispersive spectrometers, change dipole moments during molecular vibrations, Interferogram and its Fourier Transformation, Far-IR, Mid-IR, Near IR spectral regions, optical windows: KBr, CsI pellet technique, Paraffin mulls, ZnSe, CaF<sub>2</sub> windows; Total internal reflectance based devices,

**Raman Spectroscopy:** Construction of the instrument, use of lasers as excitation source, Rayleigh scattering and Raman scattering, polarizability & molecular vibrations, Stokes lines and anti-Stokes lines, Resonance Raman technique, interpretation of a Raman spectra. Using FTIR and Raman spectra to determine geometry of a molecule, intermolecular interactions.

## UNIT III

### Resonance Techniques

**Nuclear Magnetic Resonance (NMR):** Construction of the instrument, basic principles, magnetic nuclei and Larmor precession, chemical shift and intensities of lines, spin orbit coupling, fluxionality, recording the spectrum, NMR of paramagnetic molecules, contact and dipolar shifts, <sup>15</sup>N, <sup>19</sup>F, <sup>31</sup>P NMR, NMR of heavy nuclei, Solid State- NMR

**Electron Paramagnetic Resonance (EPR) or Electron Spin Resonance (ESR):** Construction of the instrument, basic principles, the g-value, the hyperfine splitting, EPR of Transition metal ions: Spin Hamiltonian, spin-orbital coupling, g and A matrices, solutions to S=1/2 systems in various ligand fields, d<sup>9</sup>, d<sup>1</sup>, d<sup>5</sup> systems, S>1/2 systems, zero-field splitting – single crystal and powder spectra – spin-lattice and spin-spin relaxation, interpreting the super hyperfine coupling,

## UNIT IV

**Mössbauer spectroscopy:** the instrumental set-up, basic principles, emission of  $\gamma$ -radiation by radioactive <sup>57</sup>Co, resonant absorption of  $\gamma$ -radiation by nuclei, sensitivity of such absorption to the electronic and magnetic environment, interpreting the Mössbauer spectrum.

### SUGGESTED TEXT BOOKS

1. Instrumental Methods of Analysis, H. H. Willard, L. L. Merritt, and J. A. Dean, 6<sup>th</sup> Edition (1986),
2. Quantitative Chemical Analysis, Daniel C. Harris
3. Spectrometric Identification of Organic Compounds, 7<sup>th</sup> Edition, Robert M. Silverstein, Francis X. Webster, David Kiemle.
4. William Kemp, Organic spectroscopy, Palgrave, New York.
5. Introduction to Spectroscopy. Donald L. PaviaGeorge, S. Kriz, James A. Vyvyan.
6. Fundamentals of Analytical Chemistry by A. Skoog and M. West
7. Vogel's Hand Book of Quantitative Analysis by Longman
8. Physical methods for chemists: R.S. Drago

### SUGGESTED REFERENCE BOOKS

1. R. Wiesendanger, Scanning Probe Microscopy and Spectroscopy, Cambridge University Press, 1994.
2. Frank A. Settle, Handbook of instrumental techniques for analytical chemistry, Prince Hall, New Jersey, 1997.
3. K. W. Kolasinski, Surface science: Foundations of catalysis and nanoscience, John Wiley and Sons, West Sussex, 2002.
4. D. A. Skoog, D. M. West, F. J. Holler and S. R. Couch, Fundamentals of analytical chemistry. Brooks/Cole Cengage learning, New Delhi, 2004.
5. P. Atkins and J. de Paula, Atkins' physical chemistry, 8<sup>th</sup> Ed., Oxford University Press, New Delhi, 2008.
6. T. Pradeep, Nano: The essentials, McGraw-Hill Education, New Delhi, 2010.
7. F. Scholz, Electroanalytical Methods, Springer, 2<sup>nd</sup> Ed., 2010.

| Course Title: Green Chemistry II: Catalysis |                                                                          |                 |                       |
|---------------------------------------------|--------------------------------------------------------------------------|-----------------|-----------------------|
| Course Code                                 | DE02104 / OE02104                                                        | Credits         | 4                     |
| L + T + P                                   | 3 + 1 + 0                                                                | Course Duration | One Semester          |
| Semester                                    | Even                                                                     | Contact Hours   | 45 (L) + 15 (T) Hours |
| Methods of Content Interaction              | Lecture, Tutorials, Group discussion; self-study, seminar, presentations |                 |                       |

### Course Objectives

- To make students understand catalysis as one of the fundamental pillars of green chemistry
- To acquaint the students with the fundamentals of electrocatalysis in biological systems and water-splitting reactions
- To develop a thorough understanding of photocatalysts and their different modes of action

- To familiarize with bio-catalysis with respect to bioremediation of contaminants and to understand the enzyme-based methods of energy production

**Learning Outcomes:** After completion of the course the learners will be able to:

- Explain how biomimetic metal complexes are used as catalysts for various processes
- Design a catalyst to make a process greener
- Discuss the examples of naturally occurring photocatalytic reactions
- Underscore the importance of photocatalysts in exploiting the solar energy to drive difficult reactions
- Understand electrocatalysis with respect to water-purification and water-splitting reactions
- Discuss the bioremediation of contaminants and enzyme-catalyzed reactions for generating energy and bio-fuels

## UNIT I

**Catalysts in Green Chemistry:** Catalysis as one of the fundamental pillars of green chemistry, Catalyst design, Cu, Zn, Fe, Mn complexes as catalysts, Biomimetic Cu complexes for green oxidation of alcohols, catalysts that activate the natural oxidant hydrogen peroxide, TAML activators and its applications, aluminophosphate molecular sieve catalyst with cobalt(III) and Mn(III) ions, solid acid catalysts and the uses thereof, metal loaded silica as catalysts, Rh catalysts containing bisphosphanes and bisphosphites as chelating ligand, kaolinitic clay as catalyst.

## UNIT II

**Electrocatalysis:** Electron Transfer Process, Multi-step Reactions, Electrolysis of water, Mechanism of hydrogen evolution, Choice of electrocatalysts for h.e.r, Electrocatalytic oxidation of NAD(P) H at mediator-modified electrodes, Electrocatalysis of Hemoglobin in ionic liquid, thin films and membranes, Electrocatalytic reduction of bromate ions for water purification.

## UNIT III

**Photocatalysis:** Photocatalysis and green chemistry, photocatalytic processes in nature eg., photosynthesis, three basic ways of exploiting solar energy, photocatalysts and their modes of action, electron transfer, H abstraction, photocatalytic activity: the effect of surface area and electron-hole recombination, design of photocatalysts of high activity Photocatalysis for producing hydrogen, TiO<sub>2</sub>, other metal oxides, sulfides as photocatalysts, Photocatalysis in synthesis, photooxidation, photo-oxygenation, photoreduction, photocatalytic formation of C-C, C-N, C-X bonds, Photocatalytic remediation of environment, heterogeneous & homogeneous photocatalysis: the case of semiconductors and dyes.

## UNIT IV

**Biocatalysis:** Biocatalysis platform for green processes, Bioremediation of persistent contaminants, Microbial bioremediation, Enzymatic bioremediation, Laccases: blue enzymes for green chemistry, Laccases and chemical mediators: mimicking nature, laccases as biocatalysts for chemical reactions, optimum reaction condition for the enzyme, laccases in manufacturing industries, hyperthermophilic enzymes for biocatalysis, biophysical properties of the enzymatic breakers, Galactomannan as the supporting matrix for hydraulic fracturing of oil/gas wells, Enzymes for clean energy production, Amylolytic enzymes and bioethanol

production, Biodiesel, biohydrogen and biofuel cells, High fructose corn syrup (HFCS) production, Thermophilic esterases, biocatalysis in ionic liquids, enzyme discovery

### SUGGESTED TEXT BOOKS

1. Green Chemistry and Catalysis, R.A. Sheldon, I. Arends and U. Hanefeld, WILEY-VCH Verlag GmbH & Co. KGaA (2007).
2. Biocatalysis for Green Chemistry and Chemical Process Development, *Junhua Tao and Romas Joseph Kazlauskas*, WILEY-VCH Verlag GmbH & Co. KGaA (2011).
3. Green chemistry for chemical synthesis, *Chao-Jun Li and Barry M. Trost*, Proceedings of National Academy of Sciences (USA), year 2008, vol. 105, pages 13197–13202.
4. Advances in inorganic chemistry, Elsevier, Vol. 58, (2006).
5. Green Catalysis, *Masaya Matsuoka and Masakazu Anpo*, Wiley-VCH Verlag GmbH & Co. KGaA (2010).
6. A primer on electrocatalysis, J.O'M. BOCKRIS, J. Serb. Chem. Soc. 70 (3) 475–487 (2005)
7. Direct Electrochemistry of Hemoglobin and Its Electrocatalysis Based on Hyaluronic Acid and Room Temperature Ionic Liquid, Electroanalysis 20, 2008, No. 23, 2537 – 2542.
8. Photocatalysis. A multi-faceted concept for green chemistry, D. Ravelli, D. Dondi, M. Fagnonia and A. Albini, Chem. Soc. Rev., 2009, 38, 1999–2011.
9. Synthesis of Inorganic Solids Using Microwaves, *K. J. Rao, B. Vaidhyanathan, M. Ganguli, and P. A. Ramakrishnan*, Chemistry of Materials, 1999, 11, 882-895
10. Sonochemistry and sonoprocessing: the link, the trends and (probably) the future, Timothy J. Mason, Ultrasonics Sonochemistry 10 (2003) 175–179.

| Course Title: Nucleoside, Advances in Nucleic Acid and Proteins |                                                                          |                 |                       |
|-----------------------------------------------------------------|--------------------------------------------------------------------------|-----------------|-----------------------|
| Course Code                                                     | DE02204 / OE02204                                                        | Credits         | 4                     |
| L + T + P                                                       | 3 + 1 + 0                                                                | Course Duration | One Semester          |
| Semester                                                        | Odd                                                                      | Contact Hours   | 45 (L) + 15 (T) Hours |
| Methods of Content Interaction                                  | Lecture, Tutorials, Group discussion; self-study, seminar, presentations |                 |                       |

**OBJECTIVE:** To understand structures and functions of nucleic acid and proteins with a perspective of chemistry and biology and further integrate this for use in drug discovery and biotechnology.

### UNIT I

**Nucleoside:** Modified nucleoside as a new drugs as antiviral and anticancer agents.

**Nucleic acids:** Definition, structure and properties, different type of base pairing, double helices, Sugar-Phosphate Chain conformations, conformation of DNA, physical properties and stability of DNA. DNA replication, genetic information storage, transcription, translation, transmission and gene expression, DNA intercalation, chemical synthesis of oligonucleotides, hybridization with synthetic oligonucleotides, characterization and purification techniques, nucleic acids as molecular probes. Catalytic RNA, siRNA, micro RNA, DNA damages, mutations and repair. Modified nucleic acids: Peptide nucleic acids (PNAs), LNAs, synthesis of PNAs, doubly labeled PNAs as probes for the detection of point mutations. Single Nucleotide Polymorphism (SNPs).

## UNIT II

**Proteins:** Different strategies and methods for the production, isolation, structure determination, functional analysis and modification of proteins, analyse and interpret protein sequences and structures and use such information to predict protein function, understanding of fundamental concepts of proteomics and hands-on experience with techniques used in current proteomics. Use of protein for production and development of drugs, for biotechnological and other industrial and scientific purposes and explanation how this is facilitated by knowledge of the structure and function of proteins.

### SUGGESTED BOOKS

1. C.M. Dobson, J.A. Gerrard and A.J. Pratt., Foundations of Chemical biology, Oxford University Press 2002.
2. A. Miller and J. Tanner, Essentials of Chemical Biology, Willey & Sons Ltd. 2008. References: 1. S. L. Schreiber, T. Kapoor and G. Wess, Chemical Biology : from small molecules to systems biology and drug design, Wiley – VCH Verlag GmbH & Co. 2007.
3. S. L. Schreiber, T. Kapoor and G. Wess, Chemical Biology: from small molecules to systems biology and drug design, Wiley – VCH Verlag GmbH & Co. 2007.
4. Stryer, L.; Berg, J. M.; Tymoczko, J. L. In Biochemistry, 5<sup>th</sup> Ed. (Hardcover).
5. Lehninger Principles of Biochemistry, 5<sup>th</sup> Ed. by Nelson and Cox.
6. McLaughlin, L. W.; Wilson, M.; Ha, S. B. Use of Nucleoside Analogues to probe Biochemical Processes (a) Wojciechowski, F.; Leumann, C. J. Chem. Soc. Rev. 2011, 40, 5669. (b) Jan Stambasky, Michal Hocek and Pavel Kotovsky Chem. Rev., 2009, 109, 6729.
7. (a) Kool, E. T.; Morales, J. C.; Guckian, K. M. Angew. Chem. Int. Ed. 2000, 39, 990. (b) Kool, E. T. Acc. Chem. Res. 2002, 35, 936. (c) Teo, Y. N.; Wilson, J. N.; Kool, E. T. J. Am. Chem. Soc. 2009, 131, 3923. (d) Schweitzer, B. A.; Kool, E. T. J. Am. Chem. Soc. 1995, 117, 1863. (e) Kool, E. T. Annu. Rev. Biochem. 2002, 71, 191. (f) Jarchow-Choy, S. K.; Sjuvarsson, E.; Sintim, H. O.; Eriksson, S.; Kool, E. T. J. Am. Chem. Soc. 2009, 131, 5488.

| Course Title: Chemistry of Natural Products |                                                                          |                 |                       |
|---------------------------------------------|--------------------------------------------------------------------------|-----------------|-----------------------|
| Course Code                                 | DE02304 / OE02304                                                        | Credits         | 4                     |
| L + T + P                                   | 3 + 1 + 0                                                                | Course Duration | One Semester          |
| Semester                                    | Even                                                                     | Contact Hours   | 45 (L) + 15 (T) Hours |
| Methods of Content Interaction              | Lecture, Tutorials, Group discussion; self-study, seminar, presentations |                 |                       |

**OBJECTIVE:** To give students an awareness of the richness and diversity of plants and animal around us. To make students aware of the many pharmaceutically active products of natural origin. To learn the origin of natural products, their characterisation and synthesis.

**Course Outcome:** At the end of the course, students should be able to: The knowledge of the students is enhanced with the clear information about the natural products which are having medicinal importance.

- Identify and characterize various classes of natural products by their structures;
- Appreciate the biogenesis of many natural products of importance.

### UNIT-I

Basics of Metabolism (primary & secondary), Reactive Intermediates in Biosynthesis, Role of ATP and other important coenzyme, catabolism, anabolism, biosynthesis of terpenoids alkaloids, and other natural products.

### UNIT-II

**Terpenoids and Carotenoids:** Classification, nomenclature, occurrence and isolation. Isoprene rules. Stereochemistry of citral, farnesol, limonene, 1, 8-cineole, menthols and borneols. Correlation of configurations of terpenoids.

Structure elucidation of camphene, pinene, caryophyllene, santonin and gibberillic acid. Synthesis and biosynthesis of the following: Linalool, -terpineol, Commercial synthesis of camphor.

### UNIT-III

**Alkaloids:** Definition, nomenclature, occurrence, isolation, classification, General methods of structure elucidation. Synthesis and biosynthesis of the following alkaloids: Ephedrine, hygrine, coniine and cocaine.

### UNIT-IV

**Steroids:** Occurrence. Nomenclature, basic skeleton, Diels hydrocarbon and stereochemistry. Isolation, structure and structural elucidation of sterols and bile acids, Cholesterol.

### UNIT-V

**Porphyrins and vitamin B<sub>12</sub>:** Structure elucidation and synthesis of haemin, chlorophyll-a and vitamin-B<sub>12</sub>

**Prostaglandins:** Introduction, nomenclature, classification and biological role of prostaglandins. Synthesis of PGE<sub>1</sub> and PGE<sub>2</sub> by Corey's and Stork's approaches.

**Insect pheromones:** Introduction, classification. Pheromones in pest control. Syntheses of (one synthesis should be stereoselective synthesis)

## SUGGESTED BOOKS

1. Natural products: Their chemistry and biological significance-J. Mann, R. S. Davidson, J. B. Hobbs, D. V. Banthorpe & J. B. Harborne, Longman, UK, 1994.
2. Terpenes, J. Verghese, Tata McGraw-Hill, New Delhi, 1982.
3. Chemistry of terpenes and terpenoids, A. Newman, Academic Press, London, 1975.
4. Handbook of naturally occurring compounds Vol.II: Terpenes, T.K. Davon, A.I. Scott, Academic Press, NY, 1972.
5. Natural products chemistry Vol.I & II, K. Nakanishi, T. Goso, S. Ito, S. Natori & S. Nozoe, Academic Press, NY, 1974.
6. Total synthesis of natural products Vol.I & VI, Apsimon, John Wiley, NY, 1973-1981.
7. Organic chemistry Vol.II, I.L. Finar, 6<sup>th</sup> Edn. Longman, 1992.
8. Chemistry of natural products Vol. I & II, O. P. Aggarwal, Goel Publishing House, 6<sup>th</sup> Edn. 1982.
9. Total synthesis of natural products: The chiral approach Vol.III, S. Hanessian Pergamon Press, 1983.
10. Total synthesis of steroids, Akhaun & Titov, Jerusalem, 1969.
11. Medicinal natural products: A biosynthetic approach, P. M. Dewick. John Wiley, Chichester, 1997.
12. Chemistry of natural products: A unified approach, N. R. Krishnaswamy, University Press, India, 1999.
13. Medicinal natural products: A biosynthetic approach, P. M. Dewick. John Wiley, Chichester, 1997.

| Course Title: Agrochemicals    |                                                                          |                 |                       |
|--------------------------------|--------------------------------------------------------------------------|-----------------|-----------------------|
| Course Code                    | DE02404 / OE02404                                                        | Credits         | 4                     |
| L + T + P                      | 3 + 1 + 0                                                                | Course Duration | One Semester          |
| Semester                       | Even                                                                     | Contact Hours   | 45 (L) + 15 (T) Hours |
| Methods of Content Interaction | Lecture, Tutorials, Group discussion; self-study, seminar, presentations |                 |                       |

**OBJECTIVE:** Be familiar with several interdisciplinary areas of biochemistry, medicinal and pharmaceutical Chemistry and understanding the concepts in relation to application towards drug developments. To provide an appreciation of the importance of modern agrochemicals and the factors involved in their discovery.

### Introduction to pesticides

**i) Definition,** Classification and importance of pesticides

**ii) Pest control:** Different methods –chemical –insecticides, fungicides, herbicides, rodenticides, fumigants, chitin synthesis inhibitors and insect repellents.



### **General Mode of Action of Pesticides:**

**Insecticides:** Disrupters of the nervous system, insect growth regulators, respiration inhibitors, photosynthesis disrupters, hormone mimics, inhibitors of amino acid synthesis, inhibitors of lipid synthesis.

**Fungicides:** Membrane disrupters, inhibitors of energy production, inhibitors of cell division, inhibitors of sterol synthesis.

## **UNIT II**

### **Synthetic insecticides**

- (i) **Organochlorine insecticides**- synthesis and mode of action of methoxychlor, perthane, Dicofol, Heptachlor, Dieldrin and Endosulfan.
- (ii) **Organophosphorous insecticides** –synthesis and mode action of Phosphoric acid derivatives, phosdrin, Dichlorophos, parathion, Zolone, Aninphomethyl, TEPP and Saccharan.
- (iii) **Carbamate insecticides**- synthesis and mode of action of carbamyl, Furadan, Baygon, Aldicarb and Zectron.
- (iv) Formulation and residue analysis of organochlorine, organophosphorous and carbamate

## **UNIT III**

### **Natural insecticides and herbicides**

- i) **Insecticides of plant origin** –synthesis and importance of pyrethrins (I and II), Rotenone and Nicotine. Main constituents Neem-structural formula of Azadirachtin. Synthesis of polygodial and warbunganol (Antifeedants).
- ii) **Synthesis of pyrethroids**: synthesis of Allethrin, Bioallethrin, Cypermethrin, Fenvalerate, Decemethrin and pyrethrelone.
- iii) **Concept of Bioinsecticides** – Bacillus thuringiensis.
- iv) **Concept of pro-insecticides**-structure and mode of action of pro-pheromones and pre-pro-insecticides.
- v) **Herbicides** – synthesis, applications and mode of action of the following
  - a) Aryloxyalkyl carboxylic acid derivative: 2,4-D, MCPA, 2,4,5-T and 2,4,5-TP.
  - b) Carbamate propanil and chlorpropanil, c) Urea derivatives–Monuron and diuron, d) Aliphatic acids-Dalapon, TCA, e) Aromatic acids -2,3,6-TBA, Dicamba and Amiben, f) Nitrogen heterocyclic derivatives–Simazine, Atrazine, Amitrole, Maleic hydrazide Diquat and paraquat, g) Phenols-PCP and Dinoseb, h) Benzonitrile compounds.

## **UNIT IV**

### **Fungicides and Rodenticides**

- i) **Fungicides**: classification, synthesis application and mode of action of the following classes:
  - a) Carbamates, b) Quinones-chloranil, Dichlone and Benquinox, c) perchloromethylmercaptan derivative–captan, folpet, Difolatan and Mesulfan d) Benzimidazoles-carbendazim, Benomyl and Thiabendazole
- ii) **Rodenticides**, a) Anticoagulants-synthesis and application of warfarin, Coumatheor, Vamor, Coumatetralyl, Dicoumarol and Bromadiolol. b) Acute poisons- application of

pindone, Ratindan, Sodium Fluoroacetate, Barium fluoroacetate, Antu, Tetramine, pindone and castrix.

#### REFERENCE BOOKS:

1. Naturally occurring insecticides: M. Jacobson and D. G. Crosby.
2. Insecticides for future: Jacobson
3. Insect juvenile hormone chemistry and action: J.J Mann and M.Beroza
4. Polygodial and warburganal. Terpenoidantifeedants part-II rec, Tran, chin 106
5. Insect antifeedants: S.V.ley&P. L Toogood, chemistry in Britain, Jan 1990 P.31
6. Synthesis of Insecticides: Metcalf
7. Fungicides-Frear
8. Fungicides-Nene
9. Residue reviews vol.36: Melnikov
10. Safer insecticides: E.Hodgson
11. Crop protection agents from Nature: leonard G Copping
12. Biofertilizers and Bioinsecticides: A.M. Deshmukh
13. Insecticides and Fungicides: U Sriramulu.
14. Organo chlorine insecticides: persistent organic pollutants: F. Moriary
15. Herbicides : P. C. Kearney & D.D. Kaufnan
16. Analytical Method for pesticides: Z.Weig (Vol III)
17. Pesticide formulations: Van Valkenburg
18. Insecticides: A.S.Tahori
19. Herbicides, fungicides, formulation chemistry-A.S.Tahori
20. Environmental pollution by pesticides: C.A.Edwards
21. Pespticides managements and insecticide resistance: Watson and brown
22. Organo phosphorous pesticides M.eto

#### SUGGESTED REFERENCE BOOKS

1. Surprise! A fungus factory for taxol? Science, 260, 154, 1993.
2. Introduction to alkaloids, G.A.Cordell, Wiley, 1981.
3. Secondary metabolism, J. Mann, Clarendon Press, Oxford, 1978.
4. Chemistry and mode of action of cope protection agents, I. G. Copping, RSC, 1998.
5. Insecticides with novel modes of action, I. Ishya and D. Degheele springer, 1998.
6. Pesticides Chemistry, G. Motolcsy, M. Nadasy and V. Andriska, Elsevier.
7. Fundamentals of Medicinal Chemistry, Gareth Thomas, John Wiley & Sons Inc.
8. The Organic Chemistry of Drug Design and Drug Action, Richard Silverman, Mark W Holladay Academic Press, 2014.
9. Introduction to medicinal chemistry: How drug work, GrinauzAlex, Wiley VCH.
10. Principles of Organic Medicinal Chemistry, R. R. Nadendla, New Age International, New Delhi, 2005.

11. Modern Drug Synthesis by Jie Jack Li and Douglas S. Johnson, (Wiley Series on Drug Synthesis).
12. Strategies for Organic Drug Synthesis and Design by Daniel Lednicer, Wiley.
13. Burger's Medicinal Chemistry, Drug Discovery and Development, 7<sup>th</sup> Edition, Volume 3.

| <b>Course Title: Nano Chemistry</b>   |                                                                          |                        |                       |
|---------------------------------------|--------------------------------------------------------------------------|------------------------|-----------------------|
| <b>Course Code</b>                    | <b>DE03204 / OE03204</b>                                                 | <b>Credits</b>         | 4                     |
| <b>L + T + P</b>                      | 3 + 1 + 0                                                                | <b>Course Duration</b> | One Semester          |
| <b>Semester</b>                       | Even                                                                     | <b>Contact Hours</b>   | 45 (L) + 15 (T) Hours |
| <b>Methods of Content Interaction</b> | Lecture, Tutorials, Group discussion; self-study, seminar, presentations |                        |                       |

### Course Objectives

- To acquaint the students with the fundamentals of nanoscience and nanotechnology
- To make students learn the structure and properties of different types of nanomaterials such as luminescent, superparamagnetic and plasmonic nanocrystals etc.
- To equip the students with necessary knowledge and skills in synthesis and characterization of nanomaterials
- To develop an understanding of self-assembly and nanocatalysis
- To create awareness about applications of nanotechnology for energy generation, water purification, sensing, and healthcare

**Learning Outcomes:** After completion of the course the learners will be able to:

- Explain the nanomaterials as low dimensional systems and explain their properties
- Discuss and describe the salient features of nanomaterials such as quantum dots, plasmonic nanoparticles, superparamagnetic particles, CNTs and graphene
- Synthesize nanomaterials and characterize it using various techniques.
- Explain how the nanoparticles can be used as building blocks to create hierarchical nano/microstructures
- Discuss the origin of enhanced catalytic efficiency of nanoparticles
- Underscore the importance of nanotechnology in daily life through applications in solar cells, water purification and diagnosis and therapy

### UNIT-I

**Introduction to Nanoscience & Nanotechnology:** Introduction to the nano- the length scale, meaning of the terms nanomaterials, nanoscience and nanotechnology, nanotechnology currently in use, Historical perspectives, Nature's perspectives

Nanomaterials as low dimensional systems, classification into 2D, 1D and 0D systems. Electronic structure of such systems; Stabilization of colloidal nanoparticles, electrostatic and steric stabilization, surface functionalization of nanoparticles. Classification of nanomaterials based on their properties: Semiconductor nanoparticles: Quantum confinement effects, Quantum dots, quantum wells, quantum wires; size dependent

absorption and emission of light (luminescence); Magnetic nanoparticles: superparamagnetism, SPIONs, Giant magnetoresistance (GMR) Plasmonic nanoparticles: surface plasmon resonance, Carbon based nanomaterials: carbon nanotubes, fullerenes, graphenes, carbon dots, electron emission from CNTs, conductivity and enhanced catalytic activity compared to the same materials in the macroscopic state.

## UNIT-II

**Synthesis and Characterization of Nanomaterials:** Top-down, bottom-up approach, liquid-phase synthesis, gas-phase synthesis, vapour-phase synthesis; Stabilization of nanoparticles, Surface passivation & functionalization, bioconjugation, direct absorption, covalent coupling.

**Chemical Methods:-** Arrested precipitation, coprecipitation; Metal nanocrystals by reduction, Sol-gel synthesis; Microemulsions or reverse micelles, solvothermal synthesis; Thermolysis routes, Microwave synthesis; Sonochemical synthesis; electrochemical synthesis; photochemical synthesis, Synthesis in supercritical fluids.

**Physical Methods:** Inert gas condensation, Arc discharge, Plasma arc technique, RF plasma, Ion sputtering, Laser ablation, Laser pyrolysis, Ball Milling, Molecular beam epitaxy, Chemical vapour deposition method, Physical vapor deposition, nanolithography and nano indentation.

**Characterization:** Structural Characterization; size shape and crystal structure, Transmission electron microscopy(TEM), Scanning electron microscopy (SEM), Electron diffraction (ED), X-ray –diffraction (XRD), Atomic force microscopy (AFM), Dynamic light scattering (DLS) , Small angle X-Ray Scattering (SAXS), Neutron Scattering, Magnetic Characterization: determination magnetic susceptibility, coercivity etc, by SQUID, Vibrating sample magnetometer (VSM), Optical Characterization: UV-Vis absorption spectroscopy, Luminescence Spectroscopy.

## UNIT-III

**Self-Assembly of nanomaterials and Nanocatalysis:** Nanoparticles as building blocks, Process of self-assembly, semiconductor islands, Self-assembled Monolayers (SAMs); crystal dipole directed self-assembly of nanoparticles into one dimensional and two dimensional nanostructures, self-assembly into three dimensional superlattices, such examples of semiconductor quantum dots; Self-assembly directed by molecular recognition, protein-directed self-assembly, dendrimer directed self-assembly, nucleic acid directed self-assembly, examples of metal/metal oxides/semiconductor nanoparticles.

## UNIT-IV

**Applications of Nanotechnology:** Sensing Applications: Electrochemical sensors, Chemical sensor, physical sensors, biosensors, Nanostructured Gas Sensors, Colorimetric and fluorescent sensors for trace Contaminants in water, Detection of pesticides and explosives

**Biomedical Applications:** Luminescent NPs for imaging of cancer cells, Superparamagnetic Magnetic NPs for MRI (Magnetic resonance imaging), Noble metal NPs for imaging applications, Targeted Drug Delivery Mesoporous silica/ Polymeric nanoshells/nanoparticles for drug delivery; Liposomes and micelles as nanocarriers metal/semiconductor/polymeric nanoparticles Photodynamic therapy (PDT), Photothermal therapy (PTT) by plasmonic nanomaterials, Hyperthermia treatment by magnetic NPs.

**Energy Applications:** Solar energy for electricity production: photovoltaic nanotechnology, artificial photosynthesis Nanotechnology for: Hydrogen production, Hydrogen transport and storage, Hydrogen conversion, fuel.

### SUGGESTED TEXT BOOKS

1. A Textbook of Nanoscience and Nanotechnology, T. Pradeep, Tata McGraw Hill Education Private Limited, New Delhi (2012).
2. Nanochemistry: A Chemical Approach to Nanomaterials, Geoffrey A. Ozin, André C. Arsenault, Ludovico Cademartiri, Royal Society of Chemistry (2009).
1. Concepts of Nanochemistry, Ludovico Cademartiri, Geoffrey A. Ozin, Jean-Marie Lehn, WILEY-VCH Verlag GmbH & Co. KGaA, (2009).
2. Nano: theEssenstials, T. Pradeep, Tata McGraw Hill Education Private Limited, New Delhi (2007)
3. Environmental Applications of Nanomaterials, Glen Fryxell and Guozhong Cao, Imperial College Press, London (2007).
4. Introduction to nanotechnology, C. P. Poole Jr, F. J. Owens, 2<sup>nd</sup> edition, Wiley-India, Delhi, 2008.
5. Nanostructures and nanomaterials, G. Cao, Imperial College Press, University of Washington, USA, 2004.
1. Nanotechnology Fundamentals and applications, M. Karkare, I. K. international publishing house pvt. Ltd., Bangalore, 2008.
2. Springer Handbook of Nanotechnology, B. Bhusan, 3<sup>rd</sup> edition, Springer-Verlag, 2009.
3. Chemistry of Nanomaterials: Synthesis, Properties and Applications, CNR Rao and T. Cheetham, Wiley & Sons, 2005.
4. Nanoparticles: From Theory to Application, Günter Schmid, WILEY-VCH Verlag GmbH & Co. KGaA, (2011).
5. Nanoparticles: synthesis, stabilization, passivation, and functionalization, Ramanathan Nagarajan, T. Allan Hatton, Publisher: American Chemical Society (2008).
6. Magnetic nanoparticles, S. P. Gubin, WILEY-VCH Verlag GmbH & Co. KGaA,(2009)
7. Multifunctional Nanoparticles for Drug Delivery Applications: Imaging, Targeting, and Delivery, Sonke Svenson, Robert K. Prud'Homme, Springer (2012).

| <b>Course Title: Advanced Instrumental Techniques-II</b> |                          |                        |                          |
|----------------------------------------------------------|--------------------------|------------------------|--------------------------|
| <b>Course Code</b>                                       | <b>DE03304 / OE03304</b> | <b>Credits</b>         | 4                        |
| <b>L + T + P</b>                                         | 3 + 1 + 0                | <b>Course Duration</b> | One Semester             |
| <b>Semester</b>                                          | Odd                      | <b>Contact Hours</b>   | 45 (L) + 15 (T)<br>Hours |

|                                       |                                                                          |
|---------------------------------------|--------------------------------------------------------------------------|
| <b>Methods of Content Interaction</b> | Lecture, Tutorials, Group discussion; self-study, seminar, presentations |
|---------------------------------------|--------------------------------------------------------------------------|

### Course Objectives

- To equip the students with necessary skills in advanced instrumental techniques
- To make students proficient in various electroanalytical techniques such as cyclic voltammetry, coulometry, pulse polarography etc.
- To impart skills in thermal methods of analysis
- To make students learn the chemical composition analysis using different instrumental methods
- To acquaint students with different types of microscopy techniques such as SEM, TEM, STM, AFM, MFM, CT, OCT etc

### Learning Outcomes

After completion of the course the learners will be able to:

- Apply electroanalytical techniques such as voltammetry, polarography etc for physicochemical analysis
- Analyze thermal stability of materials and compounds using techniques such as TGA, DTA, DSC
- Determine the chemical composition of compounds/materials using CHN, XRF, ICP-AES techniques
- Perform the microstructural analysis using microscopy techniques such as SEM, TEM, AFM, STM etc.

### UNIT-I

**Electroanalytical Techniques:** Electrode Potential, Currents in Electrochemical cells, Potentiometric titrations. Electrogravimetry- faraday's laws of electrolysis, Coulometry, Coulometric titrations. Voltammetry-principle, DME-advantages, limitations, Hydrodynamic Voltammetry, Cyclic voltammetry- principle, conditions for reversible, quasi reversible and irreversible reactions. Anodic stripping voltammetry-principle and applications, Polarography, Pulsepolarography, Amperometry-titrations, different titration curves, applications, numerical problems on all these techniques.

### UNIT-II

**Thermal Methods of Analysis:** Principle, methodology and applications: thermogravimetric and differential thermal analysis, differential scanning calorimetry; Thermo-mechanical and dynamic mechanical analysis; thermometric titrations. Thermal stability of polymers, applications, decomposition patterns, decomposition reactions-examples.

### UNIT-III

**Chemical Composition Analysis:** CHN Analysis, Atomic absorption spectroscopy, Inductively Coupled Plasma-Atomic Emission spectroscopy (ICP-AES), X-ray fluorescence (XRF) technique.

### UNIT-IV

**Microscopy & Imaging Techniques:** Scanning Probe Microscopy: AFM, STM, MFM, Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM), STEM,

Vibrational Imaging: IR, Raman, CARS, SRS, X-ray Microscopy and Micro-Computed Tomography (CT) , Optical Coherence Tomography (OCT)

### SUGGESTED TEXT BOOKS

1. Instrumental Methods of Analysis, H. H. Willard, L. L. Merritt, and J. A. Dean, 6<sup>th</sup> Edition (1986),
2. Quantitative Chemical Analysis, Daniel C. Harris.
3. Spectrometric Identification of Organic Compounds, 7<sup>th</sup> Edition, Robert M. Silverstein, Francis X. Webster, David Kiemle.
4. William Kemp, Organic spectroscopy, Palgrave, New York.
5. Introduction to Spectroscopy. Donald L. Pavia, James A. Vyvyan.
6. Fundamentals of Analytical Chemistry by A. Skoog and M. West
7. Vogel's Hand Book of Quantitative Analysis by Longman
8. Physical methods for chemists: R.S. Drago

### SUGGESTED REFERENCE BOOKS

1. R. Wiesendanger, Scanning Probe Microscopy and Spectroscopy, Cambridge University Press, 1994.
2. Frank A. Settle, Handbook of instrumental techniques for analytical chemistry, Prince Hall, New Jersey, 1997.
3. K. W. Kolasinski, Surface science: Foundations of catalysis and nanoscience, John Wiley and Sons, West Sussex, 2002.
4. D. A. Skoog, D. M. West, F. J. Holler and S. R. Couch, Fundamentals of analytical chemistry. Brooks/ColeCengage learning, New Delhi, 2004.
5. P. Atkins and J. de Paula, Atkins' physical chemistry, 8<sup>th</sup> Ed., Oxford University Press, New Delhi, 2008.
6. T. Pradeep, Nano: The essentials, McGraw-Hill Education, New Delhi, 2010.
7. F. Scholz, Electroanalytical Methods, Springer, 2<sup>nd</sup> Ed., 2010.

| <b>Course Title: Green Energy Systems</b> |                                                                          |                        |                       |
|-------------------------------------------|--------------------------------------------------------------------------|------------------------|-----------------------|
| <b>Course Code</b>                        | <b>DE02504 / OE02504</b>                                                 | <b>Credits</b>         | 4                     |
| <b>L + T + P</b>                          | 3 + 1 + 0                                                                | <b>Course Duration</b> | One Semester          |
| <b>Semester</b>                           | Odd                                                                      | <b>Contact Hours</b>   | 45 (L) + 15 (T) Hours |
| <b>Methods of Content Interaction</b>     | Lecture, Tutorials, Group discussion; self-study, seminar, presentations |                        |                       |

### Course Objectives

- To make students aware of the emerging energy scenario with respect to fast depletion of fossil fuels and climate change

- To impress upon the students the need to innovate and design cleaner and greener techniques to generate energy
- To develop a thorough understanding of nuclear reactors and its use for power generation
- To make students learn the principles, design and working of electrochemical power sources
- To impart the knowledge about fuel cells and emphasize the importance of hydrogen as a fuel
- To develop a comprehensive understanding of solar cells

**Learning Outcomes:** After completion of the course the learners will be able to:

- Understand the energy crisis in relation to climate change
- Compare and contrast the green and non-green energy sources
- Explain how nuclear reactors are used for power generation
- Distinguish between primary and secondary electrochemical power sources
- Discuss the relevance of hydrogen as green fuel
- Explain the working of various types of solar cells

## UNIT I

**Overview of energy scenario:** Available energy options, their advantages and disadvantages. Environmental effects, comparative evaluation of energy options and energy needs. Fossil fuels: petroleum, natural gas and coal Origin, processing and production of value added products available current conversion technologies.

## UNIT II

**Photovoltaic cells:** Introduction, Photovoltaics (PV) in the context of global energy demand and climate change,

**The solar resource:** Spectra, insolation, diffuse vs. direct, atmospheric absorption, light absorption and charge generation, recombination in semiconductors, depletion Approximation, derivation of ideal diode law, solar cell performance output parameters, Ideal efficiency limits, Practical sources of loss, characterizing solar cell performance, Improving efficiency by reducing optical losses: texturing, anti-reflection coatings, light trapping, photon recycling, concentrating PV. Commercial Technologies based on c-Si, CdTe, organic semiconductors

## UNIT III

**Electrochemical Cells:** Electrochemical power sources theoretical background on the basis of thermodynamic and kinetic considerations. Primary cells- various types, especially magnesium and aluminium based cells, magnesium reserve batteries. Secondary cells: classification based on electrolyte type, temperature of operation on the basis of electrodes, chemistry of the main secondary batteries for electric vehicles- present status.

## UNIT IV

**Hydrogen as fuel:** Fuel cells: classification chemistry of fuel cells detailed description of hydrogen/oxygen fuel cells methanol molten carbonate solid polymer electrolyte and biochemical fuel cells. Hydrogen as fuel production (thermal, electrolysis, photolysis and photo electrochemical) storage and applications of hydrogen storage.



Solar energy conversion devices, photovoltaic cells, photo electrochemical cells, dye sensitized solar cells, semiconductor/electrolyte junctions, photocatalytic modes for fuel conversion process, and photo-biochemical options. Other methods of energy conversion: processes especially in the form of storage as chemical energy.

## SUGGESTED BOOKS

1. C. A. Vincent Modern Batteries, Edward Arnold, 1984.
2. R. Narayanan and B. Viswanathan, Chemical and Electrochemical energy systems, Orient Longmans, 1997.
3. K. Sriram, Basic Nuclear Engineering, Wiley Eastern, 1990.
4. A. S. J. Appleby and F. K. Foulkes, Fuel cell Hand Book, Von Nostrand Reinhold, 1989.
5. D. Linden, Hand book of batteries and Fuel cells, McGraw Hill Book Company, 1984.
6. T. Ohta, Solar Hydrogen energy systems, Peragamon Press, 1979.
7. M. Gratzel, Energy Resources through photochemistry and catalysis, Academic Press, 1983.
8. T. Ohta, Energy Technology, Sources, Systems and Frontiers conversions, Pergamon, 1994.
9. J. G. Speight, The chemistry and technology of petroleum, Marcel Dekker Inc. (1980).
10. J. Nelson, Physics of Solar Cells, Imperial College Press, 2003. ISBN-13: 978-1860943492.
11. Gavin J. Conibeer and Arthur Willoughby, eds., Solar Cell Materials: Developing Technologies, John Wiley & Sons, Inc., 2014, ISBN: 978-0-470-06551-8.
12. J. Poortmans and V. Arkhipov, eds., Thin Film Solar Cells: Fabrication, Characterization, and Applications, John Wiley & Sons, Ltd., 2006.

| <b>Course Title: Fundamentals of Nuclear Chemistry</b> |                                                                          |                        |                     |
|--------------------------------------------------------|--------------------------------------------------------------------------|------------------------|---------------------|
| <b>Course Code</b>                                     | <b>DE03402 / OE03402</b>                                                 | <b>Credits</b>         | <b>2</b>            |
| <b>L + T + P</b>                                       | <b>2 + 0 + 0</b>                                                         | <b>Course Duration</b> | <b>One Semester</b> |
| <b>Semester</b>                                        |                                                                          | <b>Contact Hours</b>   | <b>(L) Hours</b>    |
| <b>Methods of Content Interaction</b>                  | Lecture, Tutorials, Group discussion; self-study, seminar, presentations |                        |                     |

## Course Objectives

- To develop an understanding of nuclear and radiochemistry

**Learning Outcomes:** After completion of the course the learners will be able to:

- Explain the various phenomena taking place in the nucleus
- Understand the working of nuclear reactors
- Utilize various nuclear techniques for analytical and biomedical applications

### Unit-I

**Elementary particles:** quarks, neutrino, antineutrino; classification of nuclides based on Z and N values, nuclear stability, nuclear potential, binding energy. **Radioactivity:** Radioactive decay and equilibrium, theories of  $\alpha$ ,  $\beta^-$ ,  $\beta^+$  and  $\gamma$ -decay, ionizing radiations and their effects, internal conversion, Auger effect, Bremsstrahlung, counting techniques such as G.M. ionization and proportional counter.

### Unit-II

**Nuclear Models:** Liquid drop and Shell model-salient features, nuclear reactions: transmutation, fission and fusion, Q value, cross sections fission and fusion, fission products and fission yields; stellar nucleosynthesis

**Nuclear waste management:** Sources of radioactive waste, waste classification and characterization, techniques for waste immobilisation, disposal methods of high-level, intermediate-level and low-level wastes.

### Unit-III

**Radiation dosimetry** and radiation protection, Chemical effects of nuclear transformations; 'Hot-atom' chemistry

**Applications of radioactivity:** Radioactive techniques; tracer technique, Neutron Activation Analysis (NAA), Radioimmunoassay, Boron-Neutron Capture Therapy (BNCT), Positron Emission Tomography (PET), Proton induced X-ray Emission (PIXE), Therapeutic uses of Gamma-rays.

### Unit-IV

**Nuclear Energy:** Nuclear Energy: Principles of Fission, critical mass, Fission reactors, Thermal reactors, Fast Breeder reactors, U enrichment and processing of spent fuels. Nuclear reactor kinetics, controlled nuclear fusion, evaluation of magnetic and other confinement options for nuclear energy.

### SUGGESTED BOOKS

1. Nuclear and Radioactive chemistry; Friedlander, Kennedy and Miller; Chapters 8 and 9, 1981.
2. Essentials of Nuclear Chemistry by H.J.Arnikaar, New Age international Private Limited, New Delhi (1997)
3. Nuclear Physics, I.Kaplan, Addison –Wesley, Reading(Mass), 1963, Narosa Publishing House, New Delhi (1998)
4. Principles of Radiochemistry, H.A.C. McKay, Butterworths, London (1971)
5. Nuclear chemistry and its applications M.Haissinsky, Addison – Wesley, Reading (Mass) (1964)
6. Source Book on Atomic Energy – S. Glasstone, D.Van Nostrand, New York, 1987 (Affiliated East-West press, New Delhi, 1969).

## ME Non-Credit Course

| Basket of ME course (each 2 credits) |                                                               |
|--------------------------------------|---------------------------------------------------------------|
| 1.                                   | Lok Vidya                                                     |
| 2.                                   | Indian Language                                               |
| 3.                                   | Life Skills                                                   |
| 4.                                   | Indian Knowledge System in concerned Discipline/Subject       |
| 5.                                   | ICT & Digital Skills                                          |
| 6.                                   | Yoga, Health & Mental Wellbeing                               |
| 7.                                   | Co-curricular Activities                                      |
| 8.                                   | Human Value and ethics                                        |
| 9.                                   | Swachh Bharat Internship                                      |
| 10.                                  | Social Responsibility and Community Connect                   |
| 11.                                  | Innovation & Entrepreneurship/Internship/Apprenticeship       |
| 12.                                  | Constitutional Values                                         |
| 13.                                  | SWAYAM approved Courses                                       |
| 14.                                  | Any other course designed by the departments for this purpose |

### ME Offered by Department of Chemistry

| Course Title: Contributions of Ancient, Medieval and Contemporary Indian Chemists |                                                                          |                 |              |
|-----------------------------------------------------------------------------------|--------------------------------------------------------------------------|-----------------|--------------|
| Course Code                                                                       | ME00100                                                                  | Credits         | 0            |
| L + T + P                                                                         | 2 + 0 + 0                                                                | Course Duration | One Semester |
| Semester                                                                          | Odd                                                                      | Contact Hours   | 30 Hours     |
| Methods of Content Interaction                                                    | Lecture, Tutorials, Group discussion; self-study, seminar, presentations |                 |              |

#### Course Objectives:

- To make students well-acquainted with different modes of science communication
- To develop knowledge and skills in the field of popular and professional science communication
- To develop multimedia skills for making of short science films

#### Learning outcomes:

After completing the course, the students will be able to

- Understand the significance of communicating science through different means
- Write articles in scientific journals and popular magazines, newspapers
- Make short science films for communicating the emerging and relevant scientific topics for creating awareness in the society

## UNIT I

### Chemistry in Ancient India and Related Literature

Try to understand the chemical concepts and process of development in the following fields. Smelting of metals, Metallurgy, distillation of perfumes and fragrant ointments, making of dyes and pigments, developments of fixers, extraction of sugar, medicinal plants, ayurvedic medicines, understanding poisons, biofertilizers, chemistry laboratory and instruments, glass

Books: Caraka Saṃhitā, SuśrutaSaṃhitā, BṛhatSaṃhitā, BṛhatSaṃhitā, Rasaśāstra, Ras Ratnakar, VrihatSaṃhitā, CharakSaṃhitā etc.

## UNIT II

### Indian Chemical Scientists

Brief discussion on their biography and detailed discussion on their scientific achievements.

Nagarjuna, GovindaBhāgavat, Govindacharya, Vāgbhata, Somadeva, Yaśodhara, Somdev, Ramchandra, Varahamihari, Charak.

Acharya Prafulla Chandra Ray, Prof. Har Gobind Khorana, Prof C. N. R. Rao, Prof Darshan Ranganathan, Prof. Padmanabhan Balaram, Prof. Gautam Radhakrishna Desiraju, Prof. Anil Kakodkar, Prof Sasanka Chandra Bhattacharyya, Prof. G. S. R. Subba Rao, Prof. Sukh Dev, Prof. Ashima Chatterji, Prof. U. R. Palit, Prof. Gurubaksha Singh, Prof. Krishnasami Venkataraman, Prof. Debashis Mukherjee, Prof. Govardhan Mehta, Dr. A. V. Rama Rao etc.

## UNIT III

### Drugs, Chemical and procedure developed in Modern Era

Briefly account the modern drug and chemical procedure and advanced chemical concepts developed in modern era.

Urea Stibamine, saroglitazar (Lipaglyn), Synriam, Centchroman (Saheli), S007-867, S002-333, Risorine, Prostalyn, Brahmi, PaMZ, (PA-824, moxifloxacin, and pyrazinamide), DRF-2593 (balaglitazone) etc.

### SUGGESTED REFERENCES:

1. Subbarayappa, B.V. 1999. Indian Alchemy: its Origin and Ramifications. In *Chemistry and Chemical Techniques in India* (Ed.) Subbarayappa, B.V., Delhi: Centre for Studies in Civilizations.
2. Deshpande, Vijaya Jayant. 1998. History of Chemistry and Alchemy in India from Pre-historic to Pre- Modern Times. In *History of Indian Science and Technology a Culture AD 1000-1800* (Ed) A. Rahman. Delhi: Oxford.
3. Ray, P.C. 1909. *History of Hindu Chemistry*. Vols. I & II. London: Williams and Norgate.
4. Habib, Irfan. 2000. Joseph Needham and the History of Indian Technology. *Indian Journal of History of Science* 35(3): 245-274.
5. History of Chemistry in ancient and Medieval India: Incorporating the History of Hindu Chemistry , by Acharya Prafulla Chandra Ray, P. Ray , B.C. Guha, 2014, ChowkhambaKrishnadas Academy

6. Chemistry and Chemical Techniques in India, B. V. Subbarayappa.

| <b>Course Title: Science Communication</b> |                                                                          |                        |              |
|--------------------------------------------|--------------------------------------------------------------------------|------------------------|--------------|
| <b>Course Code</b>                         | <b>ME00200</b>                                                           | <b>Credits</b>         | <b>0</b>     |
| <b>L + T + P</b>                           | 2 + 0 + 0                                                                | <b>Course Duration</b> | One Semester |
| <b>Semester</b>                            | Odd                                                                      | <b>Contact Hours</b>   | 30 Hours     |
| <b>Methods of Content Interaction</b>      | Lecture, Tutorials, Group discussion; self-study, seminar, presentations |                        |              |

**Course Objectives:**

- To make students well-acquainted with different modes of science communication
- To develop knowledge and skills in the field of popular and professional science communication
- To develop multimedia skills for making of short science films

**Learning outcomes:**

After completing the course, the students will be able to

- Understand the significance of communicating science through different means
- Write articles in scientific journals and popular magazines, newspapers
- Make short science films for communicating the emerging and relevant scientific topics for creating awareness in the society

**Unit I**

**Fundamentals of Science Communication**

Introduction to science communication: who communicates science, why be a science communicator, Professional and popular science communication, communications amongst scientists, different modes of professional communications: peer-reviewed papers, conferences/symposia and other events; the need for popularization of science amongst people, Science writing – newspapers, magazines, books, etc. Science broadcasting – radio, TV, Science museums – international science center movement; Science events – science cafes, science festivals, etc., Science on the web – move into multi-media Effect of medium, Reach of the medium.

**Unit II:**

**Skills for Science Communication**

Thinking skills, writing skills and presentation skills ; recognition, collection and analysis of research materials; argumentation, listening and constructive dialogue, relating personal experience to the ideas, tools and values of academic research; use of multimedia tools for science communication

**Unit III**

**Popular and Professional Science Communication**

**Popular science communication:** Direct and indirect public communications, Popular science magazines, science films; Benefits of science communication to the general public, examples of popular magazines, tv programs on health, agriculture etc, satellite images,

weather forecasting, etc, interactive mobile apps and the enhanced public health, safety and productivity; Science Museums as place for exhibition and interactive playground.

### **Professional science communication:**

Science writing as storytelling, the opening, closing and the internal structure, paragraphs, sentences and the flow, condensing and energizing writing; scientific paper writing and proposal writings, preparing posters for a conference, preparing a conference talk, making good illustrations using multimedia tools

## **Unit IV**

### **Scientists, Society, Policy makers and the media**

Scientific research, public communication and formulation of science policies by the government, examples of nuclear power plants, GM crops etc.; Making of a scientific policy, assessing the risk, dealing with environmental groups and other public interest organizations; dealing with media, tackling the climate communication challenge, other challenges in science policy making.

### **SUGGESTED REFERENCES:**

1. Scientific Writing and Communication: Papers, Proposals, and Presentations 2<sup>nd</sup> Edition, Angelika Hofmann Oxford university press
2. Writing Science: Joshua Scimel, oxford Univ. press, 2012
3. J. Gregory and S. Miller, Science in Public: Communication, Culture & Credibility (New York: Plenum/Perseus/Basic Books, depending on the date
4. Bell, P., Lewenstein, B. V, Shouse, A. W., & Feder, M. A.(2009). Learning Science in Informal Environments: People, Places, and Pursuits. Washington, DC: The National Academies Press.
5. Brake, M. & Weitkamp, E. (Eds.), Introducing Science Communication. London, UK: Palgrave Macmillan.
6. Holliman, R., Thomas, J., Smidt, S., Scanlon, E., & Whitelegg, L. (2009). Practising science communication in the information age: Theorising professional practices Oxford, UK: Oxford University Press.
7. Bennet, D.J., Jennings, R.C., (2011), Successful Science Communication, Cambridge University Press, New York
8. Bowater, L, Yeoman, K. (2012), Science Communication- A Practical Guide to Scientists, Wiley-Blackwell, UK
9. Schiele, B, Michel, C, Shunke, S., Science Communication in the World: Practices, Theory and Trends, Springer Sciences Business Media, Dordrecht, Germany
10. Cottrell, S. (2005). Critical thinking skills-Developing effective analysis and argument. Palgrave Macmillan. Basingstoke, UK: