

**(Abstract)**

The Revised Scheme, Syllabus and Model Question Papers of M.Sc. Chemistry (Material Science) Programme –University Department CBCSS- implemented w.e.f. 2020 Admission - Orders issued

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ACADEMIC C SECTION

Acad/C4/3139/2013

Dated: 24.12.2020

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- Read:-1. The Minutes of the meeting of the Syndicate held on 26.10.2019, vide item No. 2019.676
2. U.O.No.ACAD C3/22373/2019. dated 08.10.2020
  3. U.O.No.Acad/C3/22373/2019, dated 12.11.2020
  4. THE Minutes of the meeting of the Department Council, dated 18.11.2020
  5. Letter from the Head, Dept. of Chemistry Dtd. 16.12.2020, along with the revised Scheme, Syllabus & Model Question Papers of the M.Sc. Chemistry (Material Science) programme CBCSS

**ORDER**

1. The meeting of the Syndicate held on 26.10.2019 resolved vide paper read (1) above to revise the Scheme and Syllabus of all Post Graduate programmes under the Choice Based Credit Semester System (CBCSS) in the Schools/Departments of University with effect from 2020 admission.

2. Subsequently, the Curriculum Committee was reconstituted as per paper read (2) above to monitor and co-ordinate the working of the Choice based Credit Semester System.

3. Accordingly, the Revised Regulations for P.G. programmes under Choice Based Credit Semester System were implemented in the Schools/Departments of the University with effect from 2020 admission as per paper read (3) above.

4. Further, the Department Council, vide paper read (4) above approved the revised Scheme, Syllabus and Model Question papers of the M.Sc. Chemistry (Material Science) programme Under Choice Based Credit Semester System, for implementation in Department of Chemistry, w.e.f 2020 admission.

5. Thereafter, the revised Scheme, Syllabus & Model Question papers of the M.Sc. Chemistry (Material Science) programme (CBCSS) prepared in line with the revised Regulations for Choice Based Credit Semester System and duly scrutinised by the Subject expert, was forwarded by the Head, Department of Chemistry, vide paper read (5), for implementation with effect from 2020 admission.

6. The Vice Chancellor after considering the matter in detail and in exercise of the powers of the Academic Council conferred under section 11 (1) Chapter III of Kannur University Act 1996, accorded sanction to implement the revised Scheme, Syllabus and Model Question Papers of the M.Sc. Chemistry(Material Science)programme under Choice Based Credit Semester System,

offered in the Department of Chemistry, Swami Anandatheertha Campus, Payyannur of the University, with effect from 2020 admission, subject to reporting to the Academic Council.

7.The revised Scheme, Syllabus and Model Question Papers of M.Sc. Chemistry(Material Science) programme (CBCSS), with effect from 2020 admission are uploaded in the University website.([www.kannuruniversity.ac.in](http://www.kannuruniversity.ac.in))

Orders are issued accordingly.

Sd/-

**BALACHANDRAN V K**  
**DEPUTY REGISTRAR (ACAD)**  
For REGISTRAR

To: Head, Dept. of Chemistry  
Swami Anandatheertha Campus, Payyannur. P.O, Edat, Kannur - 670327

Copy To: 1. The Examination Branch (through PA to CE).  
2. PS to VC / PA to PVC / PA to R  
3. DR / AR I/ AR II (Acad).  
4. The Computer Programmer (for uploading in the Website)  
5. SF / DF /FC

Forwarded / By Order

*[Signature]*  
SECTION OFFICER



*[Signature]*

Appendix to Acad/C4/3139/2013

Dated: 24.12.2021

# **KANNUR UNIVERSITY**

**Regulation, Scheme and Syllabus**

**for**

**M.Sc. PROGRAMME**

**in**

**Chemistry**

**( *Materials Science* )**

**Choice Based Credit Semester System**

**w.e.f 2020 Admission**

**KANNUR UNIVERSITY**

**School of Chemical Sciences**

# KANNUR UNIVERSITY

## REGULATIONS FOR POST GRADUATE PROGRAMMES UNDER CHOICE BASED CREDIT SEMESTER SYSTEM IN THE DEPARTMENTS/SCHOOLS EFFECTIVE FROM 2020 ADMISSION

### 1. SCOPE

- 1.1 These Regulations shall apply to all the Post Graduate programmes, including P.G. Diploma and Certificate Courses conducted by the Departments/Schools of Kannur University
- 1.2 Choice based Credit Semester System presupposes academic autonomy, cafeteria approach in academic environment, semester system, course credits, alphabetical grading and interdepartmental academic collaboration. There shall be a Department Council consisting of all the Permanent/Contract teachers of the Department. The Head of the Department shall be responsible for admission to all the programmes offered by the Department including conduct of entrance tests, verification of records, admission and evaluation. The Department Council will deliberate on courses and specify the distribution of credits semester wise and course wise. For each course, it will specify the number of credits for lectures, tutorials, practicals etc.
- 1.3 These regulations shall come into effect from 2020 admission onwards and supersede all other Regulations unless otherwise prescribed.

### 2. DEFINITIONS

- 2.1 Curriculum Committee means the Committee constituted by the Vice-Chancellor under these Regulations to monitor the running of Choice based Credit Semester System. One of the Senior Professors shall be the Convener of the Curriculum Committee coordinating the various academic activities
- 2.2 Department/Centre/School means Department/Centre/School instituted in the University as per Kannur University Statutes.
- 2.3 ‘**Academic Programme**’ means an entire course of study comprising its programme structure, course details, evaluation schemes etc. designed to be taught and evaluated in a teaching Department.
- 2.4 ‘**Course**’ means a segment of a Programme limited to one semester in a subject.
- 2.5 ‘**Programme Structure**’ means a list of courses (Core, Elective, and Open Elective)

that makes up an Academic Programme, specifying the syllabus, credits, hours of teaching, evaluation and examination schemes, minimum number of credits required for successful completion of the programme etc. prepared in conformity with University Rules

2.6 '**Core Course**' means a course that a student admitted to a particular programme must successfully complete to receive the degree, and which cannot be substituted by any other course.

2.7 '**Elective Course**' means an optional course to be selected by a student out of such courses offered in the same or any other Department/Centre.

2.8 '**Open Elective**' means an elective course which is available for students of all programmes, including students of same department. Students of other Departments may opt these courses subject to fulfilling of eligibility of criteria as laid down by the Department offering the course.

2.9 '**Credit**' means the value assigned to a course which indicates the level of instruction. Normally, one hour lecture per week equals 1 Credit; 2/3 hours practical class per week equals 1 credit. Credit for a practical could be proposed as part of a course or as a separate practical course

2.10 '**SGPA**' means Semester Grade Point Average calculated for individual semester.

2.11 '**CGPA**' is Cumulative Grade Points Average calculated for all courses completed by the students in the last year of the course by clubbing together SGPA of four semesters

### **3. ELIGIBILITY FOR ADMISSION**

3.1 Candidates, who have passed B.Sc Chemistry with Mathematics and Physics as complementary courses with minimum 50% marks or equivalent grade in core course.

3.2 Candidates who have passed their qualifying examination from Universities outside Kerala and candidates, who have passed their degrees with different nomenclature from the Universities within Kerala, should submit Recognition/Equivalency Certificate while seeking admission.

### **4. ADMISSION**

4.1. As per the regulations prescribed by the University Departments for each Programme from time to time. However, blind/deaf candidates are not eligible for admission to the course.

4.2 Admission to the PG programme of the University departments shall be made purely on the basis of Entrance Examination. Newspaper notification in this regard has to be made in the month of May itself. Entrance Examination is mandatory for all the departments even if the numbers of applicants are less than the sanctioned strength. If the number of candidates admitted based on the Entrance Exam is less than the sanctioned strength, the concerned department can fill the vacancy by making necessary press release by fulfilling the reservation norms on the basis of the marks obtained in the qualifying examination.

4.3 There should be uniformity in the date of starting the courses and conducting the End Semester Examination of different PG programmes of the University.

## **5. REGISTRATION**

5.1 Every Department/School shall have Permanent / Contract faculty members as Student Advisors. Each student at the time of admission will be assigned to an advisor by the Department Council. He/she will advise the student about the academic Programme and counsel on the choice of courses depending on the student's academic background and objective. The student will then register for the courses she/he plans to take for the semester before the classes begin.

5.2 The Department offering any course shall prescribe the maximum number of students that can be admitted taking into consideration the facilities available. The Department Council will be the authority to fix the optionals that can be offered for a Programme while ensuring that sufficient choice is given to each student in all semesters other than Semester 01. Elective courses for the next semester will be announced within 10 days of the end of the previous semester.

5.3 The student has to complete the prescribed prerequisites for the course before registration. The student within a maximum of 10 working days after the commencement of the classes can change the Optional Course with the consent of Head of the Department in consultation with the Advisor.

5.4 The Department shall make available to all students a bulletin listing all the courses offered in every Semester specifying the Credits, list of topics the course intends to cover, the name of the instructor, the timetable and examination schedule. This will be made available in the last week of each semester after it is approved by the Department Council, the Dean and the Vice Chancellor.

## 6. COURSE STRUCTURE

- 6.1 Three kinds of Courses are offered - Core, Elective and Open Elective Courses (including MOOC courses). Core Courses are offered by the Department conducting the Programme. Elective / Open Elective Courses are offered either by the Department conducting the Programme or by any other Department of the University or via MOOC.
- 6.2 Elective Courses are offered by the Department concerned. Open Elective Courses will be offered by other Departments/Centres/Institutions as options. Open Elective Courses can be opted in any of the Semesters during the entire Programme other than the first semester. The maximum students that can be admitted to an Open Elective Course is limited to forty (40) except for MOOC courses. If the student intake in a department is more than 40, then the maximum number of students that can be admitted to an Open Elective Course is equal to the student intake.
- 6.3 Every Course offered by the University Department is identified by a unique course code. Where first two letters denote Programme name (MS for Master of Science). Next three letters denote subject. This is followed by semester number such as 01, 02, 03,04. After semester number single alphabet stands for Core (C). Elective (E) and Open Elective course (O). The last two digits denote the serial number of the course in that category (C, E or O) in that programme. MSCHE01C02 MS – Master of Science, CHE-Chemistry 01 – First Semester C – Core 02– Serial number of the Core course of the programme
- 6.4 Any course including a core course of one Department can be offered as an Open Elective Course to students of other Departments
- 6.5 The minimum duration for completion of a two-year PG Programme is four (4) Semesters and the maximum period for completion is eight (8) Semesters from the date of registration. The minimum duration for completion of a one year PG programme in any subject is two (2) semesters and the maximum period for completion is four (4 semesters) four years from the date of registration.
- 6.6 No regular student shall register for more than 24 credits and less than 16 credits per Semester, subject to the provisions of the Programme concerned.
- 6.7 The total credits required for the successful completion of a four semester Programme will be between 72 to 80. For science subjects core credits should not exceed 70 per cent.

6.8 The Department Council shall design the Core, Elective and Open Courses including the detailed syllabus for each Programme offered by the Department. The Department Council shall have the freedom to introduce new courses and/or to modify/redesign existing Courses and replace any existing Course with a new Course to facilitate better exposure and training for the students, with the approval of the Faculty Council and the Academic Council.

## 7. EVALUATION

7.1 Evaluation of the students shall be done by the Faculty member who teaches the Course on the basis of Continuous Evaluation and an End Semester Examination. The proportion of the distribution of marks among End Semester Examination and Continuous Evaluation shall be 60:40. 10 percent of the scripts, subject to a minimum of 5 scripts per course will be valued by an External Examiner. If there is an average difference of more than 15 per cent in the marks awarded by the Internal and External Examiner, the scripts will be valued by one internal and External examiner, the scripts will be valued by one Internal and one External examiner together.

7.2 Continuous Evaluation includes Assignments, Seminars, periodic written examinations etc.

7.3 The allocation of marks for each component under Continuous Evaluation shall be in the following proportions:

| Theory  |                | Practical  |                |
|---|----------------|------------|----------------|
| Components  | % of marks     | Components | % of marks     |
| Test papers   | 40% (16 marks) | Tests      | 75% (30 marks) |
| Tutorial with viva, Seminar presentations, Discussion, Debate etc | 40% (16 marks) | Record     | 25% (10 marks) |



|                      |               |                      |    |
|----------------------|---------------|----------------------|----|
| Assignment           | 20% (8 marks) |                      |    |
| Total Internal marks | 40            | Total internal marks | 40 |

7.4 Mode of assessment i.e., administering of Test or Tutorial will be decided by individual departments

7.5 A copy of all records of Continuous Evaluation shall be maintained in electronic format in the Department and shall be made available for verification by the University.

7.5 Performance of each student in an assessment shall be intimated to him/her within two weeks of the conduct of test/ submission of assignment/ report.

## **8. CONDUCT OF THE END SEMESTER EXAMINATION**

8.1 The End Semester Examinations of each semester will be conducted by the Controller of Examinations. It will be the responsibility of the Department to maintain a sufficient balance of different levels of questions in the Question Bank. The tabulation registers of each Semester shall be prepared and maintained by the Examination Branch. There shall be a minimum of one external examiner to ensure transparency in the conduct of examinations. The external examiners will be faculty members appointed from other Colleges/Departments of this University or from other Universities. The duration of End Semester Examination shall be specified in the curriculum.

8.2 The Board of Examiners will function as the Pass Board and will be called the Subject Examination Board with the Head of the Department/or a nominee of the Vice Chancellor when there is no University Department offering that Programme as its Chair

## **9. ATTENDANCE**

9.1. The minimum attendance required for each Course shall be 60% of the total number of classes conducted for that semester. Those who secure the minimum attendance in a semester alone will be allowed to register for the End Semester Examination. Condonation of attendance to a maximum of 10 days in a Semester subject to a maximum of two spells within a Programme will be granted by the Vice-Chancellor.

Benefit of Condonation of attendance will be granted to the students on health grounds, for participating in University Union activities, meetings of the University Bodies and participation in extracurricular activities on production of genuine supporting documents with the recommendation of the Head of the Department concerned. A student who is not eligible for Condonation shall repeat the Course along with the subsequent batch.

## 10. GRADING

10.1 An alphabetical Grading System shall be adopted for the assessment of a student's performance in a Course. The grade is based on a 6 point scale. The following table gives the range of marks %, grade points and alphabetical grade.

| <b>Range of Marks %</b> | <b>Grade Points</b> | <b>Alphabetical Grade</b> |
|-------------------------|---------------------|---------------------------|
| 90-100                  | 9                   | A+                        |
| 80-89                   | 8                   | A                         |
| 70-79                   | 7                   | B+                        |
| 60-69                   | 6                   | B                         |
| 50-59                   | 5                   | C                         |
| Below 50                | 0                   | F                         |

10.2A minimum of grade point 5 (Grade C) is needed for the successful completion of a Course. A student who has failed in a Course can reappear for the End Semester Examination of the same Course along with the next batch without taking re-admission or choose another Course in the subsequent Semesters of the same programme to acquire the minimum credits needed for the completion of the Programme. There shall not be provision for improvement of CE and ESE. A student can sit the ESE again if she/he has successfully completed the CE requirements in a subsequent semester subject to the maximum durations permitted.

10.3 Performance of a student at the end of each Semester is indicated by the Semester Grade Point Average (SGPA) and is calculated by taking the weighted average of grade points of the Courses successfully completed. Following formula is used for the calculation. The average will be rounded off to two decimal places.

**CGPA =  $\frac{\text{Sum of (grade points in a course multiplied by its credit)}}{\text{Sum of Credits of Courses}}$**

**Sum of Credits of Courses**

10.4 At the end of the Programme, the overall performance of a student is indicated by the Cumulative Grade Point Average (CGPA) and is calculated using the same formula given above.

10.5. Empirical formula for calculating the percentage of marks will be

$$\% \text{ Marks} = (\text{CGPA} \times 10) + 5.$$

10.6 Based on the CGPA overall letter grade of the student and classification shall be in the following way.

| <b>CGPA</b>                     | <b>Overall Letter Grade</b> | <b>Classification</b>        |
|---------------------------------|-----------------------------|------------------------------|
| 8.5 and above                   | A+                          | First Class with Distinction |
| 7.5 and above but less than 8.5 | A                           |                              |
| 6.5 and above but less than 7.5 | B+                          | First Class                  |
| 5.5 and above but less than 6.5 | B                           |                              |
| 5 and above but less than 5.5   | C                           | Second Class                 |

10.7 Appearance for Continuous Evaluation (CE) and End Semester Evaluation (ESE) are compulsory and no Grade shall be awarded to a candidate if he/she is absent for CE/ESE or both.

10.8A student who fails to complete the Programme/Semester can repeat the full Programme / Semester once, if the Department Council permits to do so. Absence in an examination will be marked zero.

10.9 No student shall be allowed to take more than eight/twelve consecutive Semesters for completing a four/six Semester Programme from the date of enrolment.

## **11. GRADE CARD**

11.1. The Controller of Examinations shall issue the grade cards of all semesters and the consolidated grade card and certificates on completion of the programme, based on the details submitted by the Heads of the Departments concerned. This will be in digital form only.

11.2. The Grade Card shall contain the following

- a) Title of the Courses taken as Core, Elective & Open Elective.
- b) The credits associated with and grades awarded for each Course.
- c) The number of credits (Core /Elective / Open) separately earned by the student and the SGPA.
- d) The total credits (Core / Elective / Open) separately earned by a student till that Semester.

11.3. The consolidated grade statement issued on completion of the Programme shall contain the name of the Programme, the Department/School offering the Programme, the title of the Courses taken, the credits associated with each Course, grades awarded, the total credits (Core /Elective/Open) separately earned by the student, the CGPA and the class in which the student is placed. Rank Certificates will be issued based on CGPA calculated at the end of the last semester of that Programmes.

## **12. DEPARTMENT COUNCIL**

- 12.1 All the Permanent and Contract teachers of the Department shall be the members of the Department Council.
- 12.2 The Department Council subject to these Regulations shall monitor every academic programme conducted in the Department.
- 12.3 Department Council shall prescribe the mode of conduct of courses, conduct of examinations and evaluation of the students.
- 12.4 An elected student representative also may attend the department council meeting where agenda related to academic matters / research activities of students are discussed

## **13. CURRICULUM COMMITTEE**

- 13.1 There shall be a Curriculum Committee constituted by the Vice Chancellor to monitor and co-ordinate the working of the Choice based Credit Semester System.
- 13.2 A senior professor nominated by the Vice Chancellor shall be the convener of the Curriculum Committee.
- 13.3 The Committee shall consist of:
  - a) Vice-Chancellor or person nominated by VC (Chairperson)
  - b) The Convener of the Curriculum Committee (A professor of the University nominated by the Vice-Chancellor)
  - c) The Registrar -Secretary

- d) The Controller of Examinations
- e) Deans
- f) The Heads of the Departments

13.4 The term of office of the Committee shall be two years, but the Committee once constituted shall continue in office until a reconstituted committee assumes office.

#### **14. ACADEMIC GRIEVANCE REDRESSAL MECHANISM**

14.1 Committees will be constituted at the Department and University levels to look into the written complaints regarding Continuous Evaluation (CE). Department Level Committee (DLC) will consist of the Department Council, and elected student representatives who is currently a student of that Programme of study. There will be one student representative for the post graduate programmes and one student representative for the doctoral programme.

14.2 University Level Committee (ULC) will consist of the Convenor of the Curriculum Committee, the concerned Dean, the concerned Head of the Department and a nominee of the Students' Union

14.3 Department Level Committee will be presided over by the HoD. Complaints should be submitted to the Department concerned within two weeks of publication of results of Continuous Evaluation (CE) and disposed of within two weeks of receipt of complaint. Appeals to University Level Committee should be made within two weeks of the decisions taken by Department Level Committee and disposed of within two weeks of the receipt of the complaint.

14.4 Complaints unsolved by the University Level Grievance Committee shall be placed before the Vice Chancellor.

#### **15. TRANSITORY PROVISION**

15.1 Notwithstanding anything contained in these regulations, the shall for a period of one year (may be revised) from the date of coming into force of these regulations, the Vice Chancellor have the power to provide by order that these regulations shall be applied to any Programme with such modifications as may be necessary.

#### **16. REPEAL**

16.1 The Regulations now in force so far as they are applicable to programmes offered in

the University Departments and to the extent they are inconsistent with these regulations are hereby repealed. In the case of any inconsistency between the implemented regulations of Choice based Credit Semester System and its application to any independent programme offered in a University Department, the former shall prevail.

**M.Sc. DEGREE COURSE in CHEMISTRY (MATERIAL SCIENCE)**  
**under Choice Based Credit and Semester System**

**(Effective from 2020 Admission)**

**About the Department**

The School of Chemical Sciences was established in 2002 and is housed at the Payyanur Campus of the University located at Edat, Payyanur. The School is offering M.Sc Chemistry (Material Science) course and Ph.D. in Chemistry and Biochemistry. The M.Sc. course pattern is of Credit and Semester System consisting of four semesters including one semester project work. The course has designed with specialization in material science and is equivalent to the M.Sc. course in chemistry of Kannur University. The School of Chemical Sciences is having an excellent Library with latest editions of textbooks, reference books and relevant journals in chemistry and material science. Library also providing internet facility to students. The School of Chemical Sciences has academic collaboration with South Indian Universities and National Research Laboratories such as Mangalore University, Cochin University of Science and Technology and University of Calicut, Central Electrochemical Research Institute, Karaikudi, Sri Chitra Tirunal Institute of Medical Science and Technology, Thiruvananthapuram, NIIST, Trivandrum and Centre for Materials for Electronics Technology, Thrissur etc.. Fourth semester M.Sc. students carry out their project works in reputed national Institutes.

- 1 The M.Sc. degree course in Chemistry (Material Science) shall be equivalent to the M.Sc. degree course in Chemistry conducted by the Kannur University.
- 2 The course shall be offered in four semesters during a period of two academic years. Each semester will have 17-18 weeks duration. The minimum duration for completion of the course is four semesters. The maximum period for the completion of the course is eight semesters.
- 3 The course is offered at the School of Chemical Sciences, Swami Anantha Theertha Campus of Kannur University situated at Edat, Payyanur.
- 4 The course is based on Choice based Credit System. The total credit required to complete the course is fixed as 80 out of which 54 credit core courses and 26 credit electives.
- 5 The number of periods allotted per week for a topic is considered as its credit. For practical, three hours is considered as one credit. Elective courses will be offered depending on the availability of the teaching staff/resource person at that time. At least 6 students have to register for an offered elective course.
- 6 No student shall register for more than 28 credits and less than 10 credits per semester. The duration of the course shall extend to more than two years (maximum four years) for the students securing less than 12 credits in a semester.

**Course details:**

- 1 The first semester, there will be 4 core courses and one elective course. In Second and third semesters, there will be 4 core courses and 3 elective courses each. In Fourth semester, there will be 2 core courses and one elective course. An open course is offered for other department students in the fourth semester.

- 2 During the third semester, the students will have to visit a Research Institute of National repute to have an idea about the current research activities. The report of the same may be submitted to the head of the department for valuation.
- 3 During the fourth semester, each student shall carry out project work in any branches of Chemistry/ Material Science for a period of not more than six months under the supervision of a teaching staff of the department nominated by the head of the department. The project can be carried out in a research institute/industry of national repute with co-guidance from experts there. The departmental council shall make decisions regarding the project details.
- 4 A student will have to present one seminar (one credit) in the second semester. The topics of the seminar will be chosen by the student in concern with his/her tutor.
- 5 Attendance is compulsory for each course and the minimum requirement for appearing for the end semester examination shall be as per general regulations of M.Sc. programme of the University.
- 6 Open elective means an elective course which is available for students of all programmes, including students of the same department. Students of other Department will opt these courses subject to fulfilling the eligibility of criteria as laid down by the Department offering the course.
- 7 One hour per week is allotted for tutorial classes. Each student will be assigned to a teaching staff of the department as his/her advisor.

#### **Programme Specific Outcomes**

- 1 Understand how chemistry relates to the real world and be able to communicate their understanding of chemical principles to a lay audience and as well apply the knowledge when situation warrants.
- 2 Develop a better understanding of the current chemical principles, methods and theories with the ability to critically analyse at an advanced level.
- 3 Acquire solid knowledge of classical and modern experimental techniques and interpretation of results; thereby acquire the ability to plan and carry out independent projects.
- 4 Develop the qualities of time management and organization, planning and executing experiments.
- 5 Learn to search scientific literature and databases, extract and retrieve the required information and apply it in an appropriate manner.
- 6 Demonstrate proficiency in undertaking individual and/or team-based laboratory investigations using appropriate apparatus and safe laboratory practices.
- 7 Develop analytical solutions to a diversity of chemical problems identified from application contexts; critically analyse and interpret qualitative & quantitative chemical information's.
- 8 Set the scene to make use of the wide range of career options open to chemistry graduates.



### SEMESTER I

| No                      | Course Code | Topic  | Contact Hours/week |     |    | Marks |    |            | Credits   |
|-------------------------|-------------|--|--------------------|-----|----|-------|----|------------|-----------|
|                         |             |  | L                  | T/S | P  | ESE   | CE | Total      |           |
| <b>CORE COURSES</b>     |             |  |                    |     |    |       |    |            |           |
| 1                       | MSCHE01C01  | Coordination Chemistry (part I) , Nuclear Chemistry & Organometallic Chemistry | 4                  | -   | -  | 60    | 40 | 100        | 4         |
| 2                       | MSCHE01C02  | Electro Chemistry, Electrode and Phase Equilibria                              | 4                  | -   | -  | 60    | 40 | 100        | 4         |
| 3                       | MSCHE01C03  | Quantum Chemistry and Chemical bonding   | 4                  | -   | -  | 60    | 40 | 100        | 4         |
| 4                       | MSCHE01C04  | Inorganic Chemistry Practical  | -                  | -   | 12 | 60    | 40 | 100        | 4         |
| Total for core courses  |             |  | 24                 |     |    |       |    | <b>400</b> | 16        |
| <b>ELECTIVE COURSES</b> |             |  |                    |     |    |       |    |            |           |
| 5                       | MSCHE01E01  | Conceptual Organic Chemistry   | 1x4                | -   | -  | -     | -  | 100        | 4         |
| 6                       | MSCHE01E02  | Advanced Organic Synthesis   |                    |     |    |       |    |            |           |
| 7                       | MSCHE01E03  | Medicinal Chemistry  |                    |     |    |       |    |            |           |
| <b>Total</b>            |             |  |                    | -   |    |       |    | <b>500</b> | <b>20</b> |

### SEMESTER II

| No                  | Course Code | Topic                                       | Contact Hours/week |     |   | Marks |    |       | Credits |
|---------------------|-------------|---|--------------------|-----|---|-------|----|-------|---------|
|                     |             |   | L                  | T/S | P | ESE   | CE | Total |         |
| <b>CORE COURSES</b> |             |   |                    |     |   |       |    |       |         |
| 1                   | MSCHE02C05  | Reactive Organic Chemistry                  | 4                  | -   | - | 60    | 40 | 100   | 4       |
| 2                   | MSCHE02C06  | Equilibrium, Nonequilibrium and Statistical | 4                  | -   | - | 60    | 40 | 100   | 4       |

|                         |                |   |     |   |    |    |    |            |           |
|-------------------------|----------------|---|-----|---|----|----|----|------------|-----------|
|                         |                | Thermodynamics  |     |   |    |    |    |            |           |
| 3                       | MSCHE0<br>2C07 | Group Theory and Spectroscopy                                       | 4   | - | -  | 60 | 40 | 100        | 4         |
| 4                       | MSCHE0<br>2C08 | Experimental Organic Chemistry                                      | -   | - | 12 | 60 | 40 | 100        | 4         |
| Total for core courses  |                |   | 24  |   |    |    |    | 400        | 16        |
| <b>ELECTIVE COURSES</b> |                |   |     |   |    |    |    |            |           |
| 5                       | MSCHE0<br>2E04 | Coordination Chemistry - (part II) & Structural inorganic chemistry | 2x4 | - | -  | 60 | 40 | 200        | 8         |
| 6                       | MSCHE0<br>2E05 | Chemical and Electrochemical Energy Systems                         |     |   |    |    |    |            |           |
| 7                       | MSCHE0<br>2E06 | Environmental Chemistry   |     |   |    |    |    |            |           |
| 8                       | MSCHE0<br>2E07 | Seminar   | -   | 1 | -  | -  | -  | 50         | 1         |
| <b>Total</b>            |                |   | 33  |   |    |    |    | <b>650</b> | <b>25</b> |

### SEMESTER III

| No                      | Course Code    | Topic                           | Contact Hours/week |     |    | Marks |    |            | Credits |
|-------------------------|----------------|---------------------------------|--------------------|-----|----|-------|----|------------|---------|
|                         |                |                                 | L                  | T/S | P  | ESE   | CE | Total      |         |
| <b>CORE COURSES</b>     |                |                                 |                    |     |    |       |    |            |         |
| 1                       | MSCHE0<br>3C09 | Progressive Organic chemistry   | 4                  | -   | -  | 60    | 40 | 100        | 4       |
| 2                       | MSCHE0<br>3C10 | Advanced Bioinorganic Chemistry | 4                  | -   | -  | 60    | 40 | 100        | 4       |
| 3                       | MSCHE0<br>3C11 | Chemical Kinetics and Catalysis | 4                  | -   | -  | 60    | 40 | 100        | 4       |
| 4                       | MSCHE0<br>3C12 | Physical Chemistry Practical    | -                  | -   | 12 | 60    | 40 | 100        | 4       |
| Total for core courses  |                |                                 | 24                 |     |    |       |    | <b>400</b> | 16      |
| <b>ELECTIVE COURSES</b> |                |                                 |                    |     |    |       |    |            |         |
| 5                       | MSCHE0         | Analytical Chemistry            | 2x4                | -   | -  | 60    | 40 | 200        | 8       |

|       |                |                   |    |   |   |   |   |            |           |
|-------|----------------|-------------------|----|---|---|---|---|------------|-----------|
|       | 3E08           |                   |    |   |   |   |   |            |           |
| 6     | MSCHE0<br>3E09 | Polymer Chemistry |    |   |   |   |   |            |           |
| 7     | MSCHE0<br>3E10 | Biochemistry      |    |   |   |   |   |            |           |
| 8     | MSCHE0<br>3E11 | Study Tour Report | -  | - | - | - | - | 50         | 1         |
| Total |                |                   | 33 |   |   |   |   | <b>650</b> | <b>25</b> |

#### SEMESTER IV

| No                      | Course Code    | Topic                                       | Contact Hours/week |     |    | Marks |    |            | Credits   |
|-------------------------|----------------|---|--------------------|-----|----|-------|----|------------|-----------|
|                         |                |   | L                  | T/S | P  | ESE   | CE | Total      |           |
| <b>CORE COURSES</b>     |                |   |                    |     |    |       |    |            |           |
| 1                       | MSCHE0<br>4C13 | Research Project                            |                    | -   | 26 | 100   | -  | 100        | 4         |
| 2                       | MSCHE0<br>4C14 | Comprehensive Viva                          | -                  | -   | -  | 100   | -  | 100        | 2         |
| Total for core courses  |                |   | 26                 |     |    |       |    | <b>200</b> | <b>6</b>  |
| <b>ELECTIVE COURSES</b> |                |   |                    |     |    |       |    |            |           |
| 3                       | MSCHE0<br>4E12 | Inorganic and Nano Materials                | 1x4                | -   | -  | 60    | 40 | 100        | 4         |
| 4                       | MSCHE0<br>4E13 | Ceramics, Composites and inorganic polymers |                    |     |    |       |    |            |           |
| Total                   |                |   | 30                 |     |    |       |    | <b>300</b> | <b>10</b> |

#### OPEN COURSE (Offered to other department students)

|       |                |                        |     |   |   |  |  |  |   |
|-------|----------------|------------------------|-----|---|---|--|--|--|---|
| 5     | MSCHE0<br>4O01 | Contemporary Chemistry | 1x3 | - | - |  |  |  | 3 |
| Total |                |                        | 3   |   |   |  |  |  | 3 |

|                    |                         |                             |
|--------------------|-------------------------|-----------------------------|
| <b>Grant Total</b> |                         |                             |
| <b>Marks: 2100</b> | <b>Core Credits: 54</b> | <b>Elective Credits: 26</b> |

*Course code- MSCHE: Master of Science Chemistry; C: Core; E: Elective; O: Open Course (online)*

### DETAILS OF GRADING SCHEME

- An alphabetical Grading System is adopted for the assessment of a student's performance in the Course. The grade is based on a 6 point scale. The following table gives the range of marks, grade points and alphabetical grade.

| Range of Marks | Grade Points | Alphabetical Grade |
|----------------|--------------|--------------------|
| 90 – 100       | 9            | A+                 |
| 80 – 89        | 8            | A                  |
| 70 – 79        | 7            | B+                 |
| 60 – 69        | 6            | B                  |
| 50 – 59        | 5            | C                  |
| Below 50       | 0            | F (Failed)         |

- A minimum of grade point 5 (Grade C) is needed for the successful completion of a course.
- Minimum credit to be fulfilled for the successful completion of the programme is 80 credits.
- Performance of a student at the end of each Semester is indicated by the Grade Point Average (GPA) and is calculated by taking the weighted average of grade point of the Courses successfully completed. Following formula is used for the calculation. The average will be rounded off to two decimal places.

Sum of (Grade Points in a Course Multiplied by its Credit)

$$\text{GPA} = \frac{\text{Sum of (Grade Points in a Course Multiplied by its Credit)}}{\text{Sum of credits of Courses}}$$

- The overall performance of a student is indicated by the Cumulative Grade Point Average (CGPA) and is calculated using the same formula given above.
- Empirical formula for calculating the percentage of marks will be  $(\text{CGPA} \times 10) + 5$ .
- Based on the CGPA, the overall grade of the student shall be in the following way.

| CGPA                            | Overall Letter Grade | Classification of Grade      |
|---------------------------------|----------------------|------------------------------|
| 8.5 and above                   | A+                   | First Class with Distinction |
| 7.5 and above but less than 8.5 | A                    |                              |
| 6.5 and above but less than 7.5 | B+                   | First Class                  |
| 5.5 and above but less than 6.5 | B                    |                              |
| 5 and above but less than 5.5   | C                    | Second Class                 |

In the case of any inconsistency between the implemented regulations of Choice based Credit Semester system and its application to PG Programme in Chemistry (Materials Science) offered in the University Department, the former shall prevail.

## **FIRST SEMESTER**

### **MSCHE01C01: Coordination Chemistry (Part I), Nuclear Chemistry & Organometallic Chemistry**

#### **Aim and Objectives**

1. To generate the significance of Coordination chemistry, which remains as one of the primary components of Inorganic chemistry?
2. To understand and apply the concepts and theories of coordination complexes.
3. To understand the formation and stability of complexes
4. To realize the critical comparison between V.B, C.F.T and M.O theories.
5. To generate an idea regarding the structure of the nucleus, different nuclear reactions, methods of measuring radioactivity etc. in terms of modern aspects of nuclear science and induce the students to take up nuclear research in their higher studies.
6. To understand organometallic compounds including alkaline, alkaline earth, and transition metals, and sometimes broadened to include metalloids like boron, silicon, and tin, as well.

#### **Learning Outcome.**

1. The student can understand and application of coordination compounds in qualitative as well as quantitative chemical analysis.
2. By understanding the spectrochemical series, the student will be capable to distinguish between strong and weak field ligands for their further applications.
3. To calculate CFSE and thereby applying the concept in variation in ionic radii, Lattice energy, thermodynamic effects etc.
4. Upon completion of this course, the students will be able to understand how Radiation can be used to improve the quality of life in many more ways than people realize.
5. By studying this course student should realize the applications of nuclear energy which uses radioactive materials, has a variety of important applications in electricity generation, medicine, industry, agriculture, as well as in our homes.
6. Student should realize the nuclear power of our nation.
7. Learners will be capable to understand the use organometallic compounds in major industrial processes including hydrogenation, olefin metathesis, alkene polymerization, alkene oligomerization, methanol carbonylation, and hydroformylation etc.

#### **Module 1**

#### **Coordination Chemistry -1**

**18 hrs**

Introduction to Coordination Chemistry, Types of ligands and complexes. Coordination number and geometry. Isomerism: Geometrical, optical and structural isomerism. Stability of complex ions in aqueous solution: Formation constants. Stepwise and overall formation constants. Factors affecting stability of complexes. Determination of stability constants. Chelate and macrocyclic effects. Theories

of Metal Complexes, Valence bond theory and its limitations. Ligand field theory: Splitting of d orbitals in different ligand fields such as octahedral, tetragonal, square planar, tetrahedral, trigonal bipyramidal and square pyramidal fields. Jahn-Teller effect. LFSE and its calculation. Thermodynamic effects of LFSE. Factors affecting the splitting parameter. Spectrochemical series. Molecular orbital theory based on group theoretical approach and bonding in metal complexes. MO diagrams of complexes with and without Pi-bonds. Effect of Pi bonding on stability. Nephelauxetic series.

**Module 2    Nuclear Chemistry    18 hrs**

Nuclear structure, Mass and charge, Binding energy, Nuclear stability, Magic numbers, Nuclear moments, Magnetic properties of nucleus, Nuclear models: Shell, Liquid drop, Fermi gas, Collective and optical models, Radioactive equilibrium, Transient and secular equilibria, Nuclear reactions: Q-value, Semi empirical mass equation, Types of nuclear reactions, Spontaneous and induced nuclear fission, reaction cross section and critical size, Nuclear fusion, Stellar energy. Nuclear energy in India.

**Module 3    Radiation Chemistry    18 hrs**

Detection and measurement of radioactivity: Principle and working of GM, Proportional, Ionization and Scintillation counters. Interaction of gamma radiation with matter: Effects of radiation on the structure and stability of solids, Radiolysis of water, Radiation dosimetry, Fricke dosimeter. Applications of radioactivity: Tracer techniques, Rock dating, Nuclear reactors, Neutron activation analysis, Szilard Chalmers effect, Chemistry of Thorium, Uranium and Plutonium. Application of thorium in nuclear reactions.

**Module 4    Organometallic Chemistry    18 hrs**

Transition metal alkyls and aryls, routes of synthesis, stability and decomposition pathways, organo copper in organic synthesis, transition metal to carbon multiple bonded compounds, alkylidenes, alkylidynes, low valent carbenes and carbynes synthesis, nature of bond, structural characteristics and reactivity (electrophilic and nucleophilic reactions on the ligands). Transition metal- $\pi$  complexes with unsaturated organic molecules: alkenes, alkynes, allyl, diene, dienyl, arene, and trienyl complexes, fluxionality and dynamic equilibria in compounds such as  $\eta^2$  – olefin,  $\eta^3$  – allyl and dienyl complexes, catalysis by organometallic compounds: hydrogenation, hydroformylation, Monsanto Acetic Acid, Wacker process and polymerization reactions.

**References/compulsory reading**

1. *Nuclear Chemistry*, C. V. Shekar, Dominant Publishers, 2014
2. *Radiochemistry and Nuclear Chemistry*, G. R. Choppin, J.-O. Liljezin and J. Rydberg, Academic Press, 2013
3. *Sourcebook on Atomic Energy*, S. Glasstone, Van Nostrand, 1958.
4. *Essentials of Nuclear Chemistry*, H. J. Arnikaar, New Age International, 1981
5. *Nuclear Chemistry – Through Problems*, H. J. Arnikaar and N. S. Rajuvar, New Age International, 2007.
6. *Elements of Nuclear Chemistry*, R. Goplalan, Vikas Publishers, 2000.
7. *Introduction to Radiochemistry*, G. Friedlander and J. W. Kennedy, John Wiley and Sons.
8. “*Advanced Inorganic Chemistry*” F. A. Cotton and G. Wilkinson, Wiley.
9. “*Inorganic Chemistry: Principles of Structure and reactivity*” J. E. Huheey, Harper Collins

10. *Concepts and Models of Inorganic Chemistry*, B. Douglas, D. Mc Daniel and J. Alexander, John Wiley, 2013.
11. *Inorganic Chemistry*, Shriver and Atkins, Oxford University Press, 1999.
12. *Inorganic Chemistry*, A.G. Sharpe, Pearson Education, 2012.
13. *Organometallic Chemistry*, R C Mehrotra and A Singh, New Age International.

**Supplementary/ Suggested reading**

1. *Inorganic Chemistry*, K. F. Purcell and J. C. Kotz, Cengage Learning, 2010.
2. *Coordination Chemistry*, S.F.A Kettle, Longman
3. *Modern Coordination Chemistry*, E.Lewis and R.G Wilkins (Eds) Interscience.
4. *Theoretical Inorganic Chemistry*, M C Day and J Selbin, Affiliated East West Press.

**MSCHE01C02: Electro Chemistry, Electrode and Phase Equilibria**

**Aims and Objectives:**

1. To develop an understanding of non-ideality of electrolyte solutions and its effect on equilibrium constants, electrolyte solutions and solution conductivity.
2. Learn about the thermodynamics of electrochemistry, the structure of the electrode/electrolyte interface and electrode processes.
3. To know about the phase rule and its application in 3 component system

**Learning Outcomes**

1. To understand theories of electrolytes and electrochemical reactions.
2. Ascertain the application of electrochemistry in industrial fields.
3. Understand the theories and applications behind various types of analytical techniques in electrochemistry.
4. Acquire the knowledge in Phase composition and rule
5. Acquire skill in solving numerical problems.

**Module 1 Electrochemistry-I 24 hrs**

Ionic nobilities, influence of pressure and temperature on ion conductance, Walden's equation, abnormal ion conductance, Derivation of Debye-Huckel-Onsager equation, validity of Debye-Huckel-Onsager equation for aqueous and nonaqueous solution, conductance ratio and Onsager equation, dispersion of conductance at high frequencies, Debye-Falken effect, Debye-Huckel limiting law and its various forms and qualitative and quantitative tests, osmotic coefficient, ion association and dissociation constant, tripple ion and conductance minima, equilibria in electrolytes, solubility product principle, solubility in presence of common ion, activity coefficient and solubility measurement.

**Module 2 Electrochemistry-II 20 hrs**

Equilibrium Electrochemistry: Electrode potential. electrochemical cell, Concentration cell, Thermodynamic properties from EMF data, Activity and activity coefficient determination for electrolytes, Ion selective electrodes, Determination of pH, Glass electrode, potentiometric titration, Redox indicators, Storage cells

**Module 3 Electrodeics 14 hrs**

Dynamic electrochemistry: Electrical double layer electric capillary, Lippmann potential, membrane potential, electrolytic polarization, dissolution and decomposition potential, concentration polarization, theories of over voltage, Hydrogen and Oxygen over voltages, Butler-Volmer equation for simple electron transfer reaction, exchange current density, Tafel equation and its significance.

**Module 4 Phase Equilibria 14 hrs**

Phase equilibria, criteria, derivation of phase rule, Two component systems: Eutectic systems, System with congruent melting point, compounds with incongruent melting point, solid solutions,

systems with partially miscible solid phase, liquid phase are partially miscible, introduction to three-component system and its graphical representation, hydrate formation, compound formation, thermal evaporation, transition point and double salt formation, salting out effect, liquid- liquid equilibria.

#### References:

1. *Introduction to Electrochemistry*, S. Glasstone, D. Van Nostrand.
2. *Modern Electrochemistry*, J.O.M. Bockris and A.K.N. Reddy, Plenum
3. *Physical Chemistry*, Daniels and Alberty, John Wiley.
4. *An Introduction to chemical thermodynamics*, Rastogi and Misra, Vikas publishing.
5. *The Principles of Electrochemistry*, D. A. Mc Innes, Dover Publishers
6. *The Principles of Electrochemistry*, D.R. Crow, Chapman and Hall
7. *Theoretical electrochemistry*, L.I. Anthropov, Mir publishers.
8. *Thermodynamics for chemists*, S. Glasstone, Affiliated East West publication
9. *Thermodynamics*, Lewis and Randall, Mc Graw Hill.
10. D. R. Crow, *Principles and Applications of Electrochemistry*, Blackie Academic and Professional, 4th Edn., 1994.
11. J. O. M. Bokris and A. K. N. Reddy, *Modern Electrochemistry*, Plenum Press, 1973.
12. G. W. Castellan, *Physical Chemistry*, Addison-Lesley Publishing.

#### Supplementary/ Suggested reading

1. Puri, Sharma, Pathania, *Principles of physical Chemistry* Vishal publishing company, 2013.
2. Gurdeep Raj *Advanced Physical Chemistry* GOEL Publishing House, Meerut, 2004.
3. S. Glasstone, *Introduction to Electrochemistry*, Biblio Bazar, 2011.
4. B. K. Sharma, *Electrochemistry*, Krishna Prakashan, 1985.

### MSCHE01C03: Quantum Chemistry and Chemical bonding

#### Aim and Objectives:

1. To understand atomic and molecular structure, as well as its properties.
2. To introduce the postulates of quantum mechanics and apply to simple systems.
3. To understand the concept of the uncertainty principle and interpret the wavefunction as a probability density.
4. To provide an introduction to the mathematical foundations of quantum chemistry.
5. To explore the application of quantum mechanics to understand the chemical phenomena, with special emphasis on chemical structure and bonding

#### Learning Outcomes:

Upon successful completion of this course, students will be able to:

1. Apply the postulates of quantum mechanics to simple systems, such as the particle-in-a-box, harmonic oscillator, rigid rotor, and hydrogenic atoms.
2. Solve the Schrödinger equations for simple systems
3. Derive the variational principle and use it to calculate properties for simple systems .
4. Use perturbation theory to calculate properties for simple systems
5. Explain the quantum mechanical nature of the chemical bond.

#### Module 1

#### Quantum chemistry- I

18 hrs

Classical mechanics and its limitations –need of quantum mechanics, Max Planck’s quantum theory of radiation, Heisenberg’s uncertainty principle, Schrodinger wave mechanics, physical meaning of wave function, well behaved functions, orthonormality of wave functions , elements of operator algebra, Eigen functions and Eigen values, Hermitian operators, the postulates of quantum mechanics, time dependent and time independent Schrodinger equations. Quantum mechanics of translational



motion, particle in a one and three-dimensional boxes, degeneracy, quantum mechanics of vibrational motion, one-dimensional harmonic oscillator, comparison of classical and quantum mechanical results, quantum mechanics of rotational motion, particle on a ring-rigid rotator, the wave function in spherical polar co-ordinates. Legendre polynomials, spherical harmonics, polar diagrams.

**Module 2** **Quantum chemistry -II** **18 hrs**

Quantum mechanics and potential energy of Hydrogen like atoms, the wave equation in spherical polar coordinates, solution of the  $R, \theta, \phi$  equations. Need of approximate methods in quantum chemistry, variation method, ground states of Hydrogen and Helium atoms, perturbation method, ground state of Helium atom, electron spin and atomic structure, spin functions and operators, Pauli's exclusion principle, Slater determinantal wave functions, spin orbit interactions, Quantization of angular momentum, quantum mechanical operators corresponding to angular momentum in polar coordinates, Russel-Saunders terms and coupling schemes.

**Module 3** **Chemical Bonding -I** **18 hrs**

Born-Oppenheimer approximation, essential principles of the MO method, MO treatment of Hydrogen molecule and the  $H_2^+$  ion, valence bond treatment of ground state of hydrogen molecule, MO treatment of homonuclear diatomic molecules,  $Li_2$ ,  $Be_2$ ,  $N_2$ ,  $O_2$ ,  $O_2^+$ ,  $O_2^-$ ,  $F_2$  and heteronuclear diatomics,  $LiH$ ,  $CO$ ,  $NO$ ,  $HF$ , correlation diagrams, noncrossing rules, spectroscopic term symbols for diatomic molecules. Theorems in chemical bonding: The Virial theorem, The Hellmann – Feynman theorem.

**Module 4** **Chemical Bonding -II** **18 hrs**

Theory of directed valency, hybridization and geometry of molecules( methane, water, ethane, acetylene), HMO theory of linear conjugated systems (ethane, allyl systems, butadiene) and its bond order, charge density and free valency calculations, HMO theory of cyclic conjugated systems(cyclobutadiene, benzene), introduction to metallic bonding, introduction to hydrogen bonding.

**References /compulsory readings**

1. *Fundamentals of Quantum chemistry*, R Anantharaman, Macmillan.
2. *Introduction to Quantum Mechanics*, L. Pauling and W.B. Wilson, McGraw Hill.
3. *Introductory Quantum chemistry*, A.K. Chandra, Tata McGraw Hill.
4. *Molecular Quantum Mechanics*, P.W. Atkins, R.S. Friedmann, Oxford University Press.
5. *Quantum chemistry*, D.A. McQuarrie, University Science Books.
6. *Quantum chemistry*, I. N. Levine, Pearson Education
7. *Quantum chemistry*, R K Prasad, New Age International
8. *Computational Methods in the Chemical Sciences*, A.F. Carley and P.H. Morgan, Eillis Horwood
9. *Theoretical Inorganic Chemistry*, M. S. Day and J. Selbin.

**Suggested and Supplementary readings:**

1. *Quantum Chemistry and Spectroscopy*, T. Engel, Pearson Education.
2. *Quantum Chemistry and Spectroscopy* M.S. Pathania, (Problems & Solutions), Vishal Publications.
3. *Quantum Mechanics in Chemistry*, M. W. Hanna, Benjamin, 3rd Edn.

**MSCHE01C04: Inorganic Chemistry Practical**

**Course Objectives:**

1. To explore the basic chemistry in aqueous medium, solubility product, color, texture, solubility, group chemistry etc. of mixture some rare earth and common inorganic salts.(cations only)

2. To explore the chemistry of complex formation and their stability.
3. To apply the principle and application of Beer Lambert's law.

**Learning outcome:**

1. Detect the cations present in unknown inorganic sample.
2. Expertise in complexometric titrations will help the students to analyse the water quality parameters such as hardness and also in their future research.
3. Expertise in colorimetric experiments will be much useful for the students in their future research for handling similar advanced equipments.

**Module 1 Mixture separation 54 hrs**

Separation and identification of four metal ions of which two are rare/less familiar such as Tl, W, V, Se, Te, Ti, Ce, Th, Zr, U, Mo and Li. (6 Experiments)

**Module 2 Volumetric estimations 40 hrs**

Estimations using EDTA- Ca, Cu, Fe, Ni, Co, (4 Nos.)

**Module 3 Colorimetric determinations & estimation of binary mixtures 68 hrs**

Colorimetric determinations of Cr, Fe, Ni and Mn. (4 Nos.).

Estimation of binary mixtures of metal ions in solution by volumetric, gravimetric, colorimetric and electro analytical methods for the following Cu, Ni, Fe, ZnMg, Ca, Ba, Cr<sub>2</sub>O<sub>7</sub> etc.

Preparation of complexes.

**Module 4 Analysis of ores/alloys and separation of binary mixtures 54 hrs**

Analysis of some typical ores and alloys.

Ion exchange separation of binary mixtures of metal ions.

NPK estimation and pH determination of soil and fertilizer.

**Reference:**

1. *A Text Book of Quantitative Inorganic Analysis*, A.I.Vogel, Longman
2. *Analysis of Minerals and Ores of Rare Elements*, W.R.Schoder and A.R. Powell
3. *Experimental Inorganic Chemistry*, W.G. Palmer.
4. *Hand Book of Preparative Inorganic Chemistry –Vol I & II*, G. Brauer
5. *Preparative Inorganic Reactions* N.L. Jolly (Ed)
6. *Quantitative Chemical Analysis*, I.M. Kolthoff and E.M. Sanderson
7. *Quantitative Chemical Analysis*, D. Levie, Tata Mc Graw Hill

**Supplementary/ Suggested reading**

1. *Semimicro Qualitative analysis*, Ramanujam.
2. *Vogel's Qualitative Inorganic Analysis*, Svehla, Pearson Education
3. *Vogel's Textbook of Quantitative Chemical Analysis*, Menham, Pearson Education

**MSCHE01E01: Conceptual Organic Chemistry**

**Aims and Objectives:**

1. To predict and explain patterns of the theory of organic chemistry
2. To understand and apply the concepts of organic chemical structure
3. To learn the bonding and stability of organic molecules
4. To have an idea of stereochemistry, and its applications
5. To learn the reactions based on photo energy
6. To study about the concerted type of reactions

**Learning Outcomes:**

1. The student can explain localized and delocalized chemical bondings, resonance, bond energy, polarizability, MOT, HMOT, aromaticity, anti, homo, non,- aromaticities, aromaticity

of heterocycle rings, fused rings, charged rings and annulenes

- The student can apply thermodynamics and kinetics of organic reactions, Hammett plots and limitations of and deviations from Hammett plots. Electronic and steric effects. Influence of structural features on acidity, basicity and reactivity of organic compounds.
- The student can illustrate classical and non-classical carbocations, chemistry of enolates and enamines, addition and insertion reactions, rearrangement reactions of carbenes
- The applications of stereo selective synthesis, asymmetric synthesis, chiral auxiliaries, methods of asymmetric induction is possible
- The student will be able to explain the reactivity in acyclic compounds. Stereochemistry of organic compounds other than carbon centre, enantiomeric and diastereomeric excess, stereochemistry of cyclohexane, fused rings and bridged compounds
- The student can apply optical rotation and optical rotatory dispersion, circular dichroism, Cotton effect and their application in assigning configuration and conformation, octant and axial haloketone rules.
- The student will be able to explain photochemical reactions, photo addition, photo oxidation, photo rearrangement, photochemistry of carbonyl compounds, alkenes and dienes, pericyclic reactions, classification, chelotropic, group transfer and ene reactions.

**Module 1 Theoretical Organic Chemistry 18 hrs**

Localized and delocalized chemical bondings, resonance, bond energy, polarizability, MOT, HMOT and its applications, Aromaticity, anti, homo, non-, aromaticities, aromaticity of heterocycle rings, fused rings, charged rings and annulenes, Limitations of and deviations from Hammett plots. Electronic and steric effects. Influence of structural features on acidity, basicity and reactivity of organic compounds

**Module 2 Reactive intermediates 18 hrs**

Carbocations: Generation, structure, detection, stability and reactions of carbocations, Classical and non-classical carbocations. Carbanions: formation, stability and structure of carbanions, chemistry of enolates and enamines. Carbenes, Benzyne and Nitrenes: structure and generation of carbenes, addition and insertion reactions, rearrangement reactions of carbenes. Structure of nitrene, generation and reactions of nitrene and related electron deficient nitrogen intermediates. Formation and reactions of benzyne. Free radicals: Generation, stability and applications of radicals.

**Module 3 Stereochemistry 18 hrs**

Introduction to isomerism: Chirality of molecules devoid of chiral centres: allenes, spirans, helicenes, restricted rotation and asymmetry, Atrop isomerism. Molecules with planar chirality: annulenes, cycloalkanes, metallocenes. Reactivity in acyclic compounds. Stereochemistry of organic compounds other than carbon centre, enantiomeric and diastereomeric excess, stereochemistry of cyclohexane, fused rings and bridged compounds. Stereo selective synthesis, asymmetric synthesis, chiral auxiliaries, methods of asymmetric induction. Introduction to optical rotation and optical rotatory dispersion, circular dichroism, Cotton effect and their application in assigning configuration and conformation, octant and axial haloketone rules.

**Module 4 Photochemistry and Pericyclic reactions 18 hrs**

Organic photochemistry: photochemical reactions, photo addition, photo oxidation, photo rearrangement, photochemistry of carbonyl compounds, alkenes and dienes, Photochemistry of aromatic compounds Barton and Hoffman-Lofferty reactions, applications, Pericyclic reactions: classification, cycloadditions, electrocyclic, sigmatropic, chelotropic and group transfer reactions, the ene- reactions, applications

**References:**

1. *A Guidebook to Mechanisms in Organic Chemistry*, P. Sykes, Pearson Education
2. *Advanced Organic Chemistry*, Jerry March, Wiley Interscience
3. *Organic Chemistry, Vol I and II*, I.L. Finar, Pearson Education
4. *Organic Chemistry*, Y. Brice, Pearson Education
5. *Principles of organic Synthesis*, R.O.C Norman, J.M.C. Frnsz, ELBS
6. *Reactive Intermediates*, C. J. Moody and W.H. Whitham, Oxford University Press
7. *Stereochemistry of organic compounds*, E.L. Eliel, Orient Longman
8. *Introduction to stereochemistry*, K. Mislow, Dower Publications
9. *Organic stereochemistry*, M.J.T. Robinson, Oxford Publications
10. *The search of organic reaction pathways*, P. Sykes, John Wiley & Sons

#### **Supplementary and suggested reading:**

1. *Organic Chemistry, Jonathan Clayden, Stuart Warren, Nick Greeves, Oxford University Press*
2. *Advanced organic chemistry, Vol I and II, Francis A. Carey and Richard J. Sundberg. Plenum Press*
3. *Organic Chemistry, T. W. Graham Solomons, Wiley*

### **MSCHE01E02: Advanced Organic Synthesis**

#### **Aims and Objectives:**

1. To learn the new synthetic methods of organic chemistry
2. To know about the latest reagents used in organic synthesis
3. To study the various types of functional group reactions
4. To learn advanced reactions mechanisms in organic chemistry
5. To understand the applications of transition metal catalysts in organic synthesis

#### **Learning Objectives:**

1. The student can understand the methodology for four and five group synthesis
2. The learner can apply stereoselective synthesis
3. The learner can explain the reactions of organometallic reagents of lithium, magnesium, copper, chromium and iron
4. The student will be able to study synthesis, reactivity and studies of metal carbonyls
5. The learner can explain Pauson Khand reaction, Vollhardt reaction, Dotz reaction
6. The student can evaluate the use of organoiron complexes for stereospecific synthesis of substituted cyclic compounds
7. The learner can understand the use of Palladium in organic synthesis,

#### **Module 1                                      New reagents in organic synthesis-I                                      24 hrs**

Retrosynthetic analysis, methodology for four and five group synthesis: terminology associated with, prostereoisomerism, homo, enantio, diastereo ligands and faces, stereoselective synthesis. Organometallic reagents of lithium, magnesium, copper, chromium and iron, ylides of sulfur and nitrogen, Tebbe’s reagent. Protecting groups, protection of hydroxyl, carboxyl, carbonyl, amino groups. Protection of carbon-carbon multiple bonds. Illustration of protection and deprotection in synthesis.

#### **Module 2                                      New reagents in organic synthesis-II                                      24 hrs**

Metal carbenes, synthesis, reactivity, analogy with ester groups for oxy carbenes, cycloaddition reactions of metal carbenes, synthesis of fused ring systems, Dotz reaction, mechanism of ring formation, application in targeted organic synthesis. Application of cobalt carbonyls in organic synthesis, Pauson Khand reaction and cyclopentenone synthesis, Vollhardt reaction.

**Module 3 Transition Metal catalysts in organic synthesis-I 10 hrs**

Pearson reaction, use of organoiron complexes for stereospecific synthesis of substituted cyclic compounds. Use of arene chromium tricarbonyl complexes in organic synthesis, the stereo effect of piano-stool structure, enhancement of arene electrophilicity and acidity of side chain. Chirality of arene chromium complexes and asymmetric synthesis.

**Module 4 Transition Metal catalysts in organic synthesis-II 14 hrs**

Palladium in organic synthesis, addition of organopalladium to unsaturated compounds, application to organic synthesis, stereochemical implications, Heck reaction, applications in synthesis. Use of zirconium and other late transition metals in addition to enyne type compounds, metallacycle formation and synthetic utility.

**References:**

1. *Advanced Organic Chemistry, Part A and B*, F. A. Carey and R. I. Sundberg, Plenum Press
2. *Principles and Applications of Organotransition Metal Chemistry*, J. P. Collman, L. S. Hegehus, J. R. Norton, and R. G. Finke, University Science Books
3. *Organic Synthesis*, Michael B. Smith, McGraw Hill
4. *Polar rearrangements*, L. M. Harwood, Oxford University Press
5. *Guidebook to Organic Synthesis*, R. K. Mackie and D. M. Smith, ELBS.
6. *Organotransition Metal Chemistry, Application to Organic Synthesis*, S. G. Davies, Pergamon Press.
7. *Designing Organic Synthesis*, S. Warren, John Wiley, 1978.

**Suggested / Supplementary Readings**

1. *Principles of Organic Synthesis*, R.O.C. Norman, J.M. Coxon, Chapman and Hall
2. *Organic Chemistry*, Clayden, N. Greeves, S. Warren, Oxford University Press
3. *Modern methods in organic synthesis*, W. Carruthers, Cambridge University Press

**MSCHE01E03: Medicinal chemistry**

**Aim and Objectives**

1. General structural features of agents belonging to the therapeutic class
2. Relevant physicochemical properties
3. Relevant chemical reactions/synthetic pathways for selected drugs
4. Structural influences on mechanism of pharmacologic action (structure-activity relationship)
5. Structural influences on pharmacologic/toxicological/therapeutic profiles. The gained knowledge is the basis for the following courses: Medicinal chemistry 2, Drug Metabolism, Pharmacology and Pharmaceutical Analysis.

**Teaching Outcomes**

1. Student will be able to: 1. Recognize the drug structure and predict its pharmacologic action;
2. Recognize the drug physico-chemical and stereochemical features;
3. Determine the pharmacophore;
4. Describe the mechanism of action, use and mode of application of the selected drugs on the basis of their structure;
5. Describe and perform synthesis of the drugs and determine the reaction yield.

**Module 1 Medicinal chemistry-I 12 hrs**

Concepts of medicinal chemistry, importance of chemistry in pharmacy, molecular pharmacology, physico-chemical properties of drugs such as solubility, partition coefficient, ionisation, acidic/basic properties, stereochemical properties etc.

**Module 2** **Medicinal chemistry-II** **24 hrs**  
Introduction to different classes of drugs, drug action, Drug discovery and design, SAR and QSAR, Hansch analysis, Craig plot, Free Wilson analysis, drug delivery systems, Enzyme inhibitors in medicine. Pharmacokinetics, drug absorption, distribution, metabolism and excretion, the role of nitric oxide in physiological states, General methods of drug synthesis (with paracetamol as eg.), synthesis and action of antibiotics (with penicillin as eg), antiviral agents, general anesthetics

**Module 3** **Medicinal chemistry-III** **24 hrs**  
Applications of Electrophoresis, ultra-filtration, ultracentrifugation in purification, separation and isolation. Introduction to herbal medicine, Introduction the chemistry of homeopathy, Introduction to nanomedicine. Organic medicinal chemistry: Introduction, general principle of drug action, physico-chemical properties of organic medicinal agents, chemistry of prodrugs, drugs metabolism, chemistry of sedatives, hypnotic drugs (barbiturates and non-barbiturates, introduction to psycho active drugs. Introduction to the chemistry of antibiotics

**Module 4** **Medicinal chemistry-IV** **12 hrs**  
Drug receptors, drug receptor interactions, hydrogen bonding, hydrophobic interactions, ionic interactions. Structure activity relationships, mechanism of drug action. Non specific action of drugs.

**Reference:**

1. *Fundamentals of Medicinal Chemistry*, G. Thomas, Wiley
2. *Introduction to Medicinal Chemistry*, G.L. Patrick, Oxford
3. *Medicinal Chemistry*, A. Kar, New Age
4. *Medicinal Chemistry, An introduction*, G. Thomas, Wiley
5. *Medicinal Chemistry*, D. Sriram, P. Yogeewari, Pearson, Education

**Supplementary/ Suggested reading**

1. *Principals of Organic Medicinal Chemistry*, R.R. Nadendla, New Age
2. *Basic Pharmacology* Cox, F Butterworths
3. *Pharmacology and pharmacotherapeutics*, Sataskar, R.S Bhandakan, S.D and Ainapure S.S., Popular Prakashan, Mumbai

**SECOND SEMESTER**

**MSCHE02C05: Reactive Organic Chemistry**

**Aims and objectives:**

1. To study of basic principles of organic chemistry,
2. To help the students to gain experience to predict the functional group transformations
3. To learn the simple reaction mechanisms
4. To understand the synthesis of organic molecules by multi-step synthesis strategies.
5. To help the students to understand the reaction mechanism subjects in later stages of their study

**Learning Outcomes:**

1. The student will be able to learn the basic principles of organic reactions and its effects on various circumstances and reaction conditions.
2. The student can understand the chemistry of heterocycles, their preparation methods and basic reactions
3. The student can illustrate the reaction pathways of Michael, Stobbe, Knoevenagal, Darzen, Dakin, Mannich, Heck reactions.

- The student can interpret Negishi, Sonogashira, Suzuki and Ullmann coupling reactions
- The mechanisms, driving force and applications of rearrangement reactions of type Bamberger, Beckmann, Benzilic acid, Classien, Curtus, Demjanov, Di-pi methane, Dienone-phenol, Favorskii, Fischer – Hepp, Fries, Hoffmann, Lossen, Schmidt, are studied.
- The student can understand and apply the use of inorganic reagents such as B, S, P, Si etc in organic synthesis
- The student will be able to learn about the Oxidation and Reduction reagents

**Module 1 Heterocyclic chemistry 18 hrs**

Introduction to heterocyclic compounds, synthesis and general reactions of pyridines, synthesis of quinolines, synthesis and general reactions of pyrans, synthesis of furan, thiophene and indole, general aspects of the chemistry of pyrimidines and purines, synthesis of imidazole, pyrazole and oxazole.

**Module 2 Reaction Mechanisms 18 hrs**

Mechanisms, reactivity and reactions of electrophilic and nucleophilic substitutions, Mechanism and reactivity of Carbon-Carbon and Carbon-Hetero multiple bonds, Oxidation and Reduction reactions, mechanisms of organic reactions: Michael, Stobbe, Knoevenagal, Darzen, Dakin, Mannich, Diels-Alder, Demjanov, Cannizaro, Bamberger and Heck reactions. Negishi, Sonogashira, Suzuki and Ullmann coupling reactions, Benzoin and Claisen condensations, Baeyer-Williger and Oppenauer oxidations, Birch reduction,

**Module 3 Rearrangement reactions 18 hrs**

Mechanisms and application of rearrangement reactions: Bamberger, Beckmann, Benzilic acid, Classien, Curtus, Demjanov, Di-pi methane, Dienone-phenol, Favorskii, Fischer – Hepp, Fries, Hoffmann, Lossen, Schmidt, Sommelet- Hauser, Stevens, Wagner- Meerwein, von Richer rearrangements.

**Module 4 Synthetic organic chemistry 18 hrs**

Reagents in organic synthesis: Boron, sulphur, phosphorous, Silicon, Mercury and cadmium containing reagents. Organometallic reagents in organic synthesis. Phase transfer catalysis, Synthesis and synthetic applications of crown ethers. Oxidation and Reduction reagents, Microwave organic synthesis, Applications of the Green strategies in organic synthesis, Electron transfers reactions, molecular transformations in organic synthesis, protective groups in organic synthesis.

**References:**

- Heterocyclic chemistry, Bensal Raj, New Age International*
- Heterocyclic chemistry, T. A. Jouis and K.Mills*
- Heterocyclic chemistry, Thomas L. Gilchrist, Pearson Education*
- Advanced Organic Chemistry, B. Miller, Pearson Education*
- Advanced Organic Chemistry, F.A. Carey and R. S. Sundberg, Springer*
- Advanced Organic Chemistry, Jerry March, Wiley Editions*
- Named Reactions, J.J. Li, Springer*
- Modern methods of organic synthesis, Carruthers, Cambridge*
- Principles of organic Synthesis, R.O.C Norman, J.M.C. Frsnz, ELBS*
- Organic synthesis, the disconnection approach, S. Warren, John Wiley*
- Organic synthesis: special techniques, V.K. Ahluwalia and R. Agagrwal, Narosa*
- Protective groups in organic synthesis, T.W. Greene and P.G.M. Wuts, John Wiley*

**Supplementary/ Suggested reading**

- Organic Chemistry, Louden, McGraw Hill

2. Organic Chemistry, Vol 2, I. L Finar, Longman.
3. Name reactions and reagents in organic synthesis, BP Mundy, MG Ellerd, FG favaloro Jr, Wiley Interscience

### MSCHE02C06: Equilibrium, Nonequilibrium and Statistical Thermodynamics

#### Aims and objectives:

1. The course aims to introduce the students to the concepts of classical and statistical Thermodynamics.
2. The classical and statistical treatment of permits to define the concepts of temperature, heat and entropy strictly from first principles without making use of empirical or axiomatic approach.
3. Emphasis is given so that the examples studied within the course can be easily generalized to any class of material or system the student will encounter in his career thus providing the skills required to accomplish tasks and solve problems by selecting and applying classical and statistical thermodynamic methods and tools.

#### Learning Outcomes:

1. Correlate thermodynamic properties and apply them in systems
2. Judge the degrees of freedom of systems and understand theories of irreversible thermodynamic systems.
3. Achieve basic skills required to derive thermodynamic properties
4. Has thorough knowledge on different classical and quantum mechanical distribution functions
5. Can explain the procedures for deriving the relation between thermodynamic parameters such as pressure, temperature, entropy and heat capacity from the distribution functions.

#### **Module 1                          Classical Thermodynamics                          24 hrs**

Nernst Heat theorem, apparent exception to third law, application of third law, Absolute entropy, residual entropy, Henry's Law, Maxwell relation and significance, Thermodynamic of partial derivative by Jacobians method, Euler's relation, thermodynamic equation of state, partial molar quantities, chemical potential and other thermodynamic functions, thermodynamics of mixing, Gibbs-Duhem-Margules equation, Lewis-Rrandall rule, fugacity in liquid mixtures, chemical affinity and other thermodynamic functions, excess thermodynamics properties.

#### **Module 2                          Irreversible Thermodynamics                          12 hrs**

Thermodynamics of irreversible process, simple examples, general theory of non equilibrium process, entropy production from heat flow, matter flow and current flow, chemical reaction, Phenomenological relations.

#### **Module 3                          Statistical Thermodynamics -I                          18 hrs**

Basic principles, permutation, probability concept, thermodynamic probability, macrostates and microstates, derivation of Boltzman distribution law, partition function, physical significance, different ensembles, distinguishable and Indistinguishable molecules, partition function and thermodynamic function, separation of partition functions, translational, rotational, vibrational and electronic partition functions, calculations of thermodynamic functions and equilibrium constants, equation of state, Sackur-Tetrode equation, statistical formulation of third law of thermodynamics.

#### **Module 4                          Statistical Thermodynamics -II                          18 hrs**

Basic idea of phase-space, heat capacity of gases, heat capacity of Hydrogen, ortho and para Hydrogens. The atomic crystals: Einstein's theory of atomic crystal, Debye's modification of



Einstein's model, The virial expression and virial coefficient, relation between virial coefficient and the cluster integrals, need for quantum statistics, Bose-Einstein statistics, Bose-Einstein distribution, theory of paramagnetism, Bose-Einstein condensation, liquid Helium, super cooled liquids, Fermi-Dirac distribution, application of free electron gas, thermionic emission, comparison of three statistics.

#### References:

1. *A course on statistical thermodynamic*, Kistin and Dorfuran- Academic 1971.
2. *Elements of statistical Thermodynamics*, L.K. Nash- Addison Wesley Publishing
3. *Elements of statistical Thermodynamics*, M.C.Gupta- New age international.
4. *An Introduction to Chemical Thermodynamics*, RP Rastogi, R R Misra, Vikas publication
5. *Thermodynamics for Chemist*, Samuel Glasttone

#### Supplementary/ Suggested reading

1. *Statistical thermodynamic*, D.A.Mc Quarrie- Harper and Row

### MSCHE02C07: Group Theory and Spectroscopy

#### Aims and Objectives:

1. To develop an understanding of the principles of molecular symmetry.
2. To provide advanced knowledge on fundamental aspects of classifying molecules based on various symmetry elements, point groups and relate their vibrational spectroscopic features.
3. To introduce some useful applications of group theory in chemistry.
4. To impart qualitative and quantitative knowledge about principles and applications of different spectroscopic techniques

#### Learning Outcomes:

Upon successful completion of this course, students will be able to:

1. Explain the symmetry of a molecule or an object.
2. Identify point groups and construct character table
3. Predict hybridisation and spectral properties based on symmetry of molecules
4. Acquire qualitative and quantitative knowledge of the fundamental concepts of various spectroscopic methods and group theoretical concept
5. Distinguish between various spectroscopic transitions

#### **Module 1** **Molecular symmetry** **18 hrs**

Molecular symmetry, groups and matrices: Symmetry elements and symmetry operations in molecules, point groups and their determinations, Schoenflies and their symbols, mathematical group, sub group, Abelian and cyclic group, group multiplication tables, classes in a group, similarity transformations of matrices, addition and multiplication of matrices, inverse of a matrix, character of a matrix, block diagonalisation, matrix form of symmetry operations, isomorphism, Matrix representation of symmetry operations, representation of groups, construction of representation using vectors and atomic orbital as basis, representation generated by cartesian coordinates positioned on the atoms of a molecule ( $H_2O$  as example)

#### **Module 2** **Group Theory** **18 hrs**

Reducible and irreducible representations, construction of irreducible representation by reduction, Great Orthogonality Theorem (GOT) (without proof), properties of irreducible representations, construction of irreducible representation using GOT, construction of character tables ( $C_2V$ ,  $C_3V$ ,  $C_4V$ ). Applications of group theory: Applications to molecular vibrations, symmetry aspects of molecular vibrations, vibrations of polyatomic molecules, selection rules for vibrational absorption, complementary character of IR and Raman spectra, determination of the number of active IR and

Raman lines, construction of hybrid orbital ( $\text{BF}_3$ ,  $\text{CH}_4$ ,  $\text{PCl}_5$  as examples), transformation properties of atomic orbital.

### Module 3

### Spectroscopy-I

18 hrs

Electromagnetic radiation: Regions of the spectrum, interaction of electromagnetic radiation with matter and its effect on the energy of molecules, selection rules, transition moment integral, microwave spectroscopy, rotational spectra of diatomic and polyatomic molecules, rigid and non-rigid rotator models, determination of bond lengths, isotope effect on rotation spectra. Vibrational energies of diatomic molecules: Interaction of radiation with vibrating molecules, determination of force constant, anharmonicity of molecular vibrations, fundamental, overtones and hot bands, degrees of freedom of polyatomic molecules and nature of molecular vibrations ( $\text{CO}_2$  and  $\text{H}_2\text{O}$  as examples), vibration-rotation spectra of diatomic and polyatomic molecules. Theory of Raman spectra (classical and quantum mechanical theory): Rotational and vibrational Raman spectroscopy, mutual exclusion principle, applications of Raman and IR spectroscopy in elucidation of molecular structure ( $\text{H}_2\text{O}$ ,  $\text{N}_2\text{O}$  and  $\text{CO}_2$  molecules as examples).

### Module 4

### Spectroscopy-II

18 hrs

Electronic spectra of diatomic molecules: Vibrational coarse structure and rotational fine structure of electronic spectrum, Franck-Condon principle, types of electronic transitions, Fortrat diagram, dissociation and predissociation. Nuclear Magnetic Resonance Spectroscopy: Magnetic properties of nuclei, theory and measurement techniques, population of energy levels, solvents used, chemical shift and its measurement, factors affecting chemical shift, relaxation methods, integration of NMR signals, spin-spin coupling, coupling constant 'j' and factors affecting it, shielding and deshielding, chemical shift assignment of major functional groups ( $\text{ABX}$ ,  $\text{AMX}$ ,  $\text{ABC}$ ,  $\text{A}_2\text{B}_2$  as examples), spin decoupling, applications of spin decoupling (with simple molecules as examples). NMR studies of nuclei other than Proton:  $^{13}\text{C}$  Chemical shift and factors affecting it,  $^{19}\text{F}$  and  $^{31}\text{P}$  NMR.

#### References/compulsory readings

1. *A Simple Approach to Group Theory in Chemistry*, S Swarnalakshmi, Universities Press
2. *Atomic and Molecular Spectroscopy*, Gupta
3. *Atomic Structure and Chemical Bonding including Molecular Spectroscopy*, Manas Chanda.
4. *Chemical Applications of Group Theory*, F A Cotton, Wiley Eastern.
5. *Fundamentals of Molecular Spectroscopy*, Banwell and McCash, Tata McGraw Hill
6. *Fundamentals of Molecular Spectroscopy*, P.S. Sindhu
7. *Group Theory and Symmetry in Chemistry*, L H Hall, McGraw Hill.
8. *Group Theory in Chemistry*, V. Ramakrishnan and M.S. Gopinathan, Vishal Publications
9. *Molecular Spectroscopy*, Barrow, McGraw Hill.
10. *Molecular Spectroscopy*, K.V. Raman,
11. *Molecular Structure and Spectroscopy*, G Aruldas, Prentice Hall.
12. *Symmetry in Chemistry*, Jaffe and Archin
13. *Theory of Atomic Spectra*, Sobelman, Alpha
14. *Vibrational Spectroscopy*, S. Narayana

#### Supplementary and suggested reading

1. *Symmetry and Spectroscopy of molecules*, K.Veera Reddy, New Age International.
2. *Molecular Symmetry and Group Theory*, Robert L. Carter, Wiley.
3. *Group Theory and Its Applications In Chemistry*, Salahuddin Kunju, G Krishnan, PHI Learning Pvt. Ltd,
4. *Introduction To Magnetic Resonance Spectroscopy ESR, NMR, NQR*. N. Sathyanarayana, IK International

## MSCHE02C08: Experimental Organic Chemistry

### Aims and objectives:

The main aim is to prepare the learner to do the laboratory works of organic chemistry. The introduction to various types of laboratory apparatus and techniques of organic synthesis and the ability for taking care of a synthesis independently, are other advantages.

### Learning outcomes:

1. The learner should be able to separate, analyze and characterize the organic compounds with common laboratory reactions and reagents
2. The student will be able to estimate the percentage content of the given substances like phenol, etc
3. The learner will be able to prepare new compounds applying many reactions and identify them using physical parameters.
4. The student can handle and carryout many laboratory identification methods such as chromatography and distillation, etc

### Module 1 Analysis of organic binary mixtures 90 hrs

Separation and identification of eight organic binary mixtures containing two components with at least two substituents in any one of the components. Recrystallization, determination of physical constants and preparation of derivatives

### Module 2 Physical Organic Experiments 20 hrs

Estimation of phenol/ aniline, estimation of glucose, equivalent weight of carboxylic acid, Estimation of lactose in milk, Determination of saponification/ iodine value of an oil

### Module 3 Preparative organic chemistry 80 hrs

1. Double stage preparation and identification of organic compounds. (Any 4)
2. Electrophilic substitution reactions–Preparations of p-bromoaniline/ p-nitroaniline/ 2,4,6-tribromophenol
3. Acetylations–Preparations of -D-glucose penta-acetate/ 2-naphthyl acetate.
4. Reactions with ring formation–Preparations of 1,2,3,4–tetrahydrocarbazole/ 1-phenyl-3-methyl-5-pyrazolone/ 7– hydroxy-4-methyl-coumarin.
5. Diazotization reactions–Preparations of iodo, chloro and azo compounds.
6. Dehydration reactions–Preparations of cyclohexene and succinic anhydride
7. Condensation reactions–Condensations involving diethyl malonate and ethyl acetoacetate. Claisen-Schmidt, Sandmayer's, Aldol and Perkin condensation reactions.

### Module 4 Organic Techniques 26 hrs

Thin layer chromatography: Monitoring of a chemical reaction, Soxhlet Extraction : natural plant leaves.

### References:

1. *A Text Book of Practical Organic Chemistry, A I Vogel, ELBS.*
2. *Advanced Practical Organic Chemistry, J. Leonard, B, Lygo and G. Procter, Nelson Thornes*
3. *Lab experiments in organic chemistry, A. Sethi, New Age international*
4. *Organic synthesis special techniques, V.K.Ahluwalia, Renu Aggarwal*
5. *Practical Organic Chemistry”, F.G. Mann and B C Saunders, Longman.*
6. *Systematic identification of organic compounds, Shriner, Hermann, Morrill, Curtin and Fuson, John Wiley*
7. *Vogel's Textbook of practical organic chemistry, B.S. Furniss, A.J. Hannaford, Pearson Education*

8. *Laboratory Manual in Organic Chemistry*–Dey & Sitaraman (Allied, New Delhi) 1992

**Suggested/ Supplementary readings:**

1. *Structural determination of organic compounds*, E. Pretsch, P. Buhlmann and C. Affolter, Springer
2. *Laboratory Manual in Organic Chemistry*–R. K. Bansal (New Age, New Delhi) 1990. 2. *Experimental Organic Chemistry*–Vol. I & II–P. R. Singh et al (TMH New Delhi) 1981
3. *Experimental Organic Chemistry*- H.D. Durst & G.E. Goke (McGraw-Hill) 1980

**MSCHE02E04: Coordination Chemistry -(Part II) & Structural inorganic chemistry**

**Aim and Objectives**

1. The course predicts and explains patterns of the various theories of spectroscopy applicable to coordination compounds, thereby understanding and applying concepts in various aspects of coordination chemistry
2. To understand the magnetic and spectral properties of transition metal complexes.
3. The objective of the course is also intended to realize the different types of reactions in transition metal complexes.
4. Introduce the learners the different types of cage, ring and cluster compounds .
5. Understand the chemistry of ring, cage and cluster compounds. Their preparation, physical and chemical properties, diverse stoichiometries and nuclearities, stability etc.
6. Wade's electron counting rules to predict trends in the stability and structures of many metal clusters.
7. Metal carbonyl cluster compounds to evaluate as catalysts for a wide range of reactions.

**Learning Outcome.**

1. Upon completion of this course, the students will be able to understand and apply the various aspects of spectroscopy to elucidate the structure of transition metal complexes.
2. By studying this course student should be capable of interpreting the electronic spectra of metal complexes for further applications.
3. By studying the reactions of metal complexes, the student can understand the applications of coordination compounds in qualitative as well as quantitative chemical analysis.
4. Use PSEPT for the prediction of structure of carboranes, metallocarboranes, metalloboranes etc.
5. Apply the concept in future research in this field.

**Module 1 Coordination Chemistry-I 18 hrs**

Optical activity of coordination compounds, ORD and CD, Cotton effect and applications. IR spectra of simple inorganic compounds and metal complexes, changes in ligand vibrations on coordination, metal ligand vibrations. NMR spectroscopy for structural investigation of diamagnetic metal complexes from chemical shift and spin-spin coupling. EPR spectra of metal complexes – hyperfine splitting, g-values, zero field splitting and Kramer's degeneracy. Applications to copper(II) complexes. Mossbauer spectra – application to iron complexes, Mossbauer effect, hyperfine interactions, isomer shift, electric quadrupole and magnetic hyperfine interactions. Importance of molar conductance measurements in coordination chemistry.

**Module 2 Coordination Chemistry-II 18 hrs**

Magnetic susceptibility measurements, Gouy method, diamagnetic corrections, spin only value, orbital contribution, spin orbit coupling, ferro and antiferro magnetic coupling, spin crossover systems, application of magnetic moment measurements for the structural determinations of transition

metal complexes. Term symbol for  $d^n$  ions, spectroscopic ground states, selection rules for d-d transitions, Orgel diagrams for transition metal complexes ( $d^1$  to  $d^9$  configuration), Tanabe-Sugano diagrams, interpretation of spectra of spin paired and spin free octahedral, distorted octahedral, tetrahedral and square planar complexes, charge transfer transitions. Electronic spectra of f-block metal complexes.

**Module 3** **Coordination Chemistry-III** **18 hrs**

Metal ligand equilibria in solutions, Stability constants, Chelate effect, Irving-William order of stability, Binary formation constants, Energy profile of a reaction, Inert and labile metal complexes, Ligand substitution reactions in octahedral metal complexes-A, D and I mechanisms. Acid hydrolysis, base hydrolysis, isomerisation and anation reactions. Substitution reactions in square planar complexes, *trans* effect - its theory and applications, *cis*-effect. Redox reactions, Inner sphere and outer sphere reactions, Complimentary and non-complimentary reactions. Reactions of coordinated ligands.

**Module 4** **Structural Inorganic Chemistry** **18 hrs**

Sulphur-nitrogen compounds: tetrasulphurtetranitride, disulphurdinitride and polythiazyl. Sulphur-phosphorus compounds: Molecular sulphides. Phosphorus-nitrogen compounds: Phosphazines, cyclo and linear phosphazines, other P-N compounds. Boron hydrides: Synthesis, reactivity, structure and bonding, Topological approach to boron hydride structure, *Styx* numbers, Icosahedral frame work, *Closo*, *Nido* and *Arachno* structures, Wades rules, Carboranes, Metalloboranes, Metallocarboranes, Boron-Nitrogen compounds, Boron nitride, Borazines. Metal clusters: Factors favouring the formation of metal-metal bonds. Metal carbonyl clusters, Anionic and hydrido clusters, LNCC and HNCC, Isoelectronic and isolobal relationships, Hetero atoms in metal clusters, Electron counting rules for HNCC, Capping rule.

**References/compulsory reading**

- 1 *Advanced Inorganic Chemistry*, F. A. Cotton and G. Wilkinson, , Wiley.
- 2 *Inorganic Chemistry- Principles of structure and reactivity*, J E Huhee, Pearson Education
- 3 *Inorganic Chemistry*, A.G. Sharpe, Pearson Education
- 4 *Inorganic Chemistry*, Shriver & Atkins, Oxford
- 5 *Chemistry of Coordination compounds*, J C Bailar, Reinhold.
- 6 *Concepts and Models of Inorganic Chemistry*, B. Douglas, D. Mc Daniel, J. Alexander,
- 7 *Concise Inorganic Chemistry* J.D. Lee, Blackwell
- 8 *Coordination Chemistry*, D Banergea, Tata McGraw Hill.
- 9 *Coordination Chemistry*, F Basolo R Johnson, Benjamin Inc.
- 10 *Coordination Chemistry*, S. F. A. Kettle, Longman.

**Supplementary/ Suggested reading**

1. *Electronic Absorption Spectroscopy and Related Techniques*, D N Sathynarayana, Universities Press.
2. *Elements of magneto Chemistry*, R L Dutta and A Syamal, S Chand & Company Ltd.
3. *Modern coordination Chemistry* , E. Lewis and R.G Wilkins (Eds.), Interscience

**MSCHE02E05: Chemical and Electrochemical Energy Systems.**

**Aim and Objectives**

Energy is a fundamental issue facing society world-wide. Electrochemical devices play an important role in energy storage and conversion, especially at certain power-levels.

1. To impart knowledge on working and performance evaluation of various energy systems

2. To facilitate analysis of energy systems using various methods and tools
3. To study about the new energy systems like fuel cells, hydrogen production and hydrogen storage

### Teaching Outcomes

Upon completion of this course, the students are expected to have the following knowledge.

1. Understand how thermodynamics, kinetics and mass transport apply to electrochemical devices
2. Understand the nature of the energized electrode and double layers.
3. Understand the two-electrode/electrolyte nature of electrochemical devices.
4. Understand the specific construction of several battery and fuel cell systems.
5. Understand battery and fuel cell charge/discharge and efficiency characteristics.

### Module 1 Introduction to chemical & electrochemical energy systems 18 hrs

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. Electrochemical power sources - theoretical background on the basis of thermodynamic and kinetic considerations.

### Module 2 Electrolyte cells & batteries 18 hrs

Primary electrolyte cells - various types, especially magnesium and aluminium based cells - magnesium reserve batteries. Secondary electrolyte cells: classification based on electrolyte type, temperature of operation on the basis of electrodes - chemistry of the main secondary batteries - Batteries for electric vehicles - present status.

### Module 3 Fuel cells-I 18 hrs

Fuel cells - classification - chemistry of fuel cells - detailed description of hydrogen/oxygen fuel cells - methanol - molten carbonate, solid polymer electrolyte and biochemical fuel cells. Solar energy conversion devices - photovoltaic cells - photoelectrochemical cells - semiconductor electrolyte junctions photocatalytic modes for fuel conversion process - photobiochemical options.

### Module 4 Fuel cells-II 18 hrs

Hydrogen as a fuel production (thermal, electrolysis, photolysis and photoelectrochemical) storage and applications of hydrogen storage. Other methods of energy conversion: processes especially in the form of storage as chemical energy.

### References:

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*, Pergamon Press, 1979.

### Supplementary/ Suggested reading

1. M. Gratzel, *Energy Resources through photochemistry and catalysis*, Academic Press, 1983.
2. T. Ohta, *Energy Technology, Sources, Systems and Frontiers conversions*, Pergamon, 1994.
3. J. G. Speight, *The chemistry and technology of petroleum*, Marcel Dekker Inc. (1980).

## MSCHE02E06: Environmental Chemistry

### Aims and Objectives:

1. To impart awareness on public health, waste management and pollution
2. To introduce basic principles of environmental chemistry like environmental processes ecosystems etc
3. To introduce various environmental policies laws and regulations that are relevant to environmental protection
4. To understand the interconnections between different sectors of the environment (soil, water, atmosphere) and the effect of human activities on these causing pollution and other impacts
5. To apply the knowledge on analytical chemistry to environmental processes and samples.

### Learning Outcomes:

1. Upon successful completion of this course, students will be able to:
2. Acquire theoretical knowledge and understanding of fundamental concepts of environmental technology
3. Understand the impact of human and natural impacts on atmosphere and ecosystem
4. Understand compounds, as well as about the chemical reactions essential for the emergence and existence of the cycling and accumulation of pollutants in the environment.
5. To apply the analytical skills previously acquired to analyse environmental processes and samples

### **Module 1 Introduction to Environmental Chemistry 18 hrs**

Introduction, important concepts, public health, public awareness, waste treatment, internal and incidental pollution, pollution control, control management, environmental policies, nature and natural process, natural resources, eco systems, social issues and the environmental pollution, environmental law and regulations.

### **Module 2 Environmental pollution-I 18 hrs**

Air pollution: chemistry, analysis, control, effect of pollution, acid rain, insecticides and pesticides, thermal pollution, depletion of ozone layer. Noise pollution: automobiles, factories, household pollution.

### **Module 3 Environmental pollution-II 18 hrs**

Water pollution: soluble metals, soaps and detergents, marine pollution, control of water pollution, Soil pollution: ground water, heavy metal poisoning, industrial pollution, agriculture pollution, radiation and radioactive pollution, Biodiversity, marine and coastal pollution.

### **Module 4 Environmental chemical analysis 18 hrs**

Instrumental methods in environmental chemical analysis, solid and liquid samples, sampling and measurements.

### References

1. *Environmental Chemistry a global perspective*, G.W. vanLoon and S.J. Duffy, Oxford University Press.
2. *Environmental chemistry*, A.K. Bhagi and G.R. Chatwal, Himalaya Publishing House
3. *Environmental Chemistry*, Ian Williams, John Wiley & Sons
4. *Environmental chemistry*, Peter O'Neill, Blackie Academics
5. *Fundamental concepts of Environmental chemistry* G.S. Sodhi, Narosa publications
6. *C. Baird, Environmental Chemistry*, W. H. Freeman and Company, 1998.
7. *D. W. Hawker, D. W. Conell, M. Warne, P. D. Vowles: Basic Concepts of Environmental Chemistry*, Lewis Publishers, Inc..1997.

### Suggested/Supplementary Reading

1. R. P. Schwarzenbach, P. M. Gschwend, D. M. Imboden: *Environmental Organic Chemistry*, J. Wiley and Sons, Inc. 1998.
2. A. G. Howard: *Aquatic Environmental Chemistry*, Oxford Science Publ., 1998.
3. S. E. Manahan: *Environmental Chemistry*, Lewis Publishers, Inc., 1994

### MSCHE02E07: Seminar

Each student has to present a seminar on a topic related to chemistry/ material science of recent trends with power point for 25-30 minutes.

### THIRD SEMESTER

#### MSCHE03C09: Progressive Organic chemistry

##### Aims and Objectives:

1. To make the student aware about the modern methods of organic synthesis
2. To introduce the UV spectroscopic techniques
3. To learn the IR spectroscopy
4. To study the NMR spectroscopy of organic molecules
5. To apply the fractionalization of organic molecules by Mass spectrum
6. To learn how to elucidate the structure of organic compounds using spectroscopic techniques
7. To learn about the natural product chemistry
8. To study the latest organic reaction techniques

##### Learning Outcomes:

1. The student is able to know about the UV spectroscopy, its effects on various parameters such as solvents, substitution, etc
2. The student can get information about the infrared spectroscopy, the factors influencing vibrational frequencies, sample techniques, solvents and group frequencies
3. The learner be able to get knowledge about the applications of IR spectroscopy, quantitative infrared analysis, Attenuated Total Reflectance and Multiple Internal Reflectance spectroscopy
4. The student will be familiar with Proton and <sup>13</sup>Carbon NMR spectroscopy, its applications to organic chemistry
5. The learner can study the theory and instrumentation of Mass spectroscopy,
6. The student will be able to determine the structure of an organic compound based on the combinations of spectroscopic techniques.
7. The student can have an idea about the Extraction and isolation of natural products, Hofmann, Emde and von Braun degradations
8. The learner will be able to digest Blanc's rule, Barbier-Wieland degradation. Oppenauer oxidation, Diel's hydrocarbon, biosynthesis of terpenes and alkaloids
9. The student will get an idea about the modern organic methods of synthesis.

##### Module 1

##### Basic Organic Spectroscopy

18 hrs

Ultraviolet and visible spectroscopy: sampling, solvent effects, limitations, applications, Woodward-Fieser method of calculations. Infrared spectroscopy: factors influencing vibrational frequencies, sample techniques, solvents, group frequencies, applications, quantitative infrared analysis, Attenuated Total Reflectance, Photo-Acoustic Spectroscopy, Multiple Internal Reflectance spectroscopy, Proton NMR spectroscopy: Chemical shift, spin-spin splitting and coupling constants, applications to organic compounds, coupling of proton to other nuclei (<sup>19</sup>F, D, <sup>31</sup>P, <sup>29</sup>Si)



**Module 2** **Advanced Organic Spectroscopy** **18 hrs**

Carbon-13 NMR spectroscopy: off-resonance and proton decoupling, Nuclear Overhauser Effect, applications, application of NMR data for stereochemical assignments, DEPT, HMQC and HSQC techniques, ESR spectroscopy. Mass spectroscopy: Theory and instrumentation, Fragmentations, application studies, McLafferty rearrangement, examples of mass spectral fragmentation of organic compounds with respect to their structure determination, Structural elucidation of organic compounds based on UV, IR, NMRs and MS data.

**Module 3** **Chemistry of natural products** **18 hrs**

Extraction and isolation of natural products, Hofmann, Emde and von Braun degradations in alkaloid chemistry, classification of Terpenoids, isoprene rules, general methods of determining the structure of terpenoids, introduction to steroids, Blanc's rule, Barbier-Wieland degradation. Oppenauer oxidation, Diel's hydrocarbon, biosynthesis of terpenes and alkaloids, analytical techniques to investigate structures, developing drugs from natural products; chemistry of key natural products

**Module 4** **Modern Organic Chemistry** **18 hrs**

Retrosynthetic Analysis: Basic principles and terminology of retrosynthesis, synthesis of aromatic compounds, one group and two group C-X disconnections, one group C-C and two group C-C disconnections, amine and alkene synthesis, important strategies of retrosynthesis, functional group transposition, important functional group interconversions. Transition metal catalysts in organic synthesis, Combinatorial chemistry, Click chemistry, Chemistry of organic electronics, Fundamentals of Supramolecular Chemistry.

**References:**

1. *Application of absorption spectroscopy of organic compounds*, J.R. Dyer, Eastern Economy edition
2. *Introduction to Organic Spectroscopy*, Pavia, Lampman and Krinz, Thomson
3. *Organic Spectroscopy* W. Kemp, Plagrove
4. *Organic structural spectroscopy*, J.B. Lambert, H.F. Shurvell, D.A. Lightner and R.G. Cooks, Prentice hall
5. *Spectrometric Identification of Organic Compounds*, R.M. Silverstein, G.C. Bassler, T.C. Morrill, John Wiley
6. *Chemistry of Natural products*, Sujata V. Bhat, BA nagasampagi, M. Shivakumar, Narosa publishing
7. *Natural products chemistry*, RR Wedekar, MR Raut, Everest publishing house
8. *Organic chemistry of natural products*, OP Qgarwal, Krishna Pralkash
9. *Organic Synthesis, The disconnection Approach*, Stuart Warren, John Wiley & Sons, 2004
10. *Carruthers, Modern Methods of Organic Synthesis*, Cambridge University Press, 1996.
11. *Kuerti and B. Czako, Strategic Applications of Named Reactions in Organic Synthesis*, Elsevier Academic Press, 2005.

**Suggested/ Supplementary readings:**

1. *F. A. Carey and R. I. Sundberg, Advanced Organic Chemistry, Part A and B, 3rd edition* Plenum Press
2. *J. Clayden, N. Greeves and S. Warren, "Organic Chemistry", Second Edition*, Oxford University Press
3. *Application of Transition Metal Catalysts in Organic Synthesis*, H. D. Verkruijse, L. Brandsma, and S.F. Vasilevsky, Springer

## MSCHE03C10: Advanced Bioinorganic Chemistry

### Course Objectives:

1. The learners should be able to realize and recognise the significance of metal and nonmetal ions in various aspects of biological system.
2. To identify the coordination complexes with respect to their role in living organisms, active site structure and functions of some transition metal ion containing metalloproteins or enzymes.

### Learning Outcomes:

At the end of the course, the learners should be able to:

1. Utilize the principles of transition metal coordination complexes in understanding their functions in biological systems.
2. Utilize the principles of transition metal coordination complexes in understanding their functions of plants.
3. Realize the significance of metal chelators used as drugs for various diseases, their methods of synthesis.
4. Generates interest to do research in this wide area useful to the human being.

### **Module 1 Introduction to bioinorganic Chemistry 18 hrs**

Introduction to Bioinorganic Chemistry, Elementary cell biology, Distribution of inorganic elements in biological systems. Essential and beneficial metal ions. Elements of life: Water, sugars, polysaccharides, amino acids, peptides, proteins, nucleosides, nucleotides, nucleic acids, lipids and phosphates. Protein synthesis and DNA replication. Coordination sites in biologically important ligands. Role of metal ions in biological functions. Biological role of some trace non-metals (B, Si, S, Se, As, Cl, Br, I), Biological importance of nitric oxide. Biomineralisation. Model compounds in biochemical studies – Biomimicry. Transport of ions across membranes: ionophores, active and passive transport,  $\text{Na}^+/\text{K}^+$  pump in biological system. Structural role of calcium, transport of calcium, intra and extra cellular calcium binding, role of calcium in blood clotting.

### **Module 2 Role of metal ions in biological systems-I 18 hrs**

Iron in biological systems, Haemoglobin (Hb) and myoglobin (Mb), transport of oxygen by heme proteins, co-operativity of oxygen binding, reversible oxygen binding, binding of CO to Hb and Mb, haemerythrin, functions of prosthetic groups, designing of synthetic blood. Storage and transport of metal ions: ferritin, transferrin, siderophores. Iron enzymes, cytochromes and their roles in biological systems. Cytochrome  $\text{P}_{450}$  and the mechanism of its activity. Copper in biological systems: ceruloplasmin, copper in oxidase activity, superoxide dismutase, structure and functions of haemocyanin, azurin, plastocyanin, Type I, II and III copper protein models.

### **Module 3 Role of metal ions in biological systems-II 18 hrs**

Role of Mn, Ni, Mo, Co, Al, Li, Cr and Zn in biology: metalloproteins as enzymes, metalloenzymes and metal activated enzymes, Zn(II) and Mg(II) containing enzymes, Zn-finger proteins, carbonic anhydrase, alcohol dehydrogenase, catalase, peroxidase, redox enzymes, DNA and RNA polymerase, DNA intercalators, vitamins and co-enzymes, vitamin  $\text{B}_{12}$ , metal toxicity and hemostasis. Diseases caused by excess and deficiency of metal ions, metals in medicine, metal ion based drugs (Pt, V and Au), metal ions as diagnostic agents, MRI imaging and contrast agents, toxicity due to non-essential elements and speciation. Chelation theory and chemotherapy, metal detoxification mechanism, thermodynamic and pharmacokinetic properties of chelating drugs in metal detoxification.

### **Module 4 Bioenergetics 18 hrs**

Bioenergetics: ATP and phosphate group transfer - a source of metabolic energy, ATP cycle and phosphate group transfer, functions of pyruvate kinase and creatine kinase, porphyrins ( $\text{H}_2\text{P}$ ) and

metalloporphyrins (MP): spectral, fluorescence and redox properties of H<sub>2</sub>P and MP, picket-fence porphyrin. Chlorophyll: PS I and PS II, model systems of water splitting and CO<sub>2</sub> reduction, Biological nitrogen fixation: nitrogenase, Fe-S clusters, Fe-protein structure, P-cluster and M-centre, nitrogenase model system.

### References/compulsory reading

- 1 *Inorganic Biochemistry*, G.L. Eichhom(Ed), Vol. 1 and 2, Elsevier, 1973.
- 2 *Advanced Inorganic Chemistry*, F. A. Cotton and G. Wilkinson, 6<sup>th</sup>Ed., Wiley, 1999.
- 3 *Biocoordination Chemistry*, D. E. Fenton, (Chemistry Primer 26), Oxford Univ. Press, 1995.
- 4 *Bioinorganic Chemistry*, L. Bertini, H. B. Gray, S. J. Lippard, and J. S. Valentine, Univ. Science Books, 1994.
- 5 *Bioinorganic Chemistry*, R.W. Hay, Ellis Harwood, 1984.
- 6 *Concepts and Models of Inorganic Chemistry*, B. E. Douglas, D. McDaniel and J. Alexander, Wiley, 2013.
- 7 *Inorganic chemistry – A Unified Approach*, W.W. Porterfield, Academic Press, 1993.
- 8 *Metal ions of Biological Systems*, H. Siegel and T. G. Spiro, Marcel-Dekker, 1980.
- 9 *Principles of Biochemistry*, A. L. Lehninger, D. L. Nelson and M. M. Cox, CBS Publishers and Distributors, 1993.
- 10 *Principles of Bioinorganic Chemistry*, S. J. Lippard & J. M. Berg, Univ. Science Books.

### Supplementary and suggested reading

- 1 *Metal in Biochemistry*, P.M. Harrison and R.J. Hoare, Chapman and Hall, 1980.
- 2 *The Inorganic Chemistry of Biological Processes*, M.N. Hughes, Wiley, 1981.
- 3 *Bioinorganic chemistry*, Asim K. Das, Books & Allied (P) Ltd.2013
- 4 *Bioinorganic and Supramolecular chemistry*, P.S Kalsi and J.P Kalsi, New age International Publishers, 2008

## MSCHE03C11: Chemical Kinetics and Catalysis

### Aims and Objectives:

1. To impart fundamental knowledge about the basic concepts of chemical kinetics.
2. To provide conceptual framework for understanding molecular reaction dynamics
3. To understand the link between reaction rates and rate constant.
4. To study the application of mathematical tools to calculate the kinetic properties of a reaction.
5. To impart knowledge of applications of catalysis.

### Learning Outcomes:

Upon successful completion of this course, students will be able to:

1. Acquire knowledge on the mechanism of chemical reactions for optimizing the experimental conditions.
2. Conduct quantitative analysis of kinetic data of chemical reactions .
3. Explain the origin of observed kinetics for simple chemical reactions.
4. Study the application of homogeneous and heterogeneous catalysis in chemical synthesis
5. Know the importance of catalytic activity at the solid surfaces

### Module 1

### Chemical Kinetics-I

24 hrs

Rate law equation: significance, determination of order of a reaction: differential, integral, isolation and half-life methods, true and false orders, determination of rate coefficient of a first order reaction by Guggenheim's methods, kinetics of complex reactions: reversible, parallel and consecutive first order reactions, Theory of unimolecular reactions: Lindman theory, steady state approximation principles, reaction involving free radicals and reactive atoms, Rice-Herzfeld mechanism, chain

reaction, branching chains, explosion, Hinshelwood mechanism of chain reactions and explosion. Thermal decomposition of organic compounds, the HI formation.

**Module 2** **Chemical Kinetics-II** **24 hrs**

Theories of reaction rate: Collision theory, transition state theory, comparison and limitations of the two theories, the kinetic and thermodynamic parameters: Significance of entropy of activation, Arrhenius equation and its temperature dependence of frequency factor, Potential energy surfaces. Salt effect: primary and secondary salt effects, influence of solvent on reaction rates. Fast reactions: Relaxation method, flow method, flash photolysis and magnetic resonance method, Reactions in solution: Factors affecting reaction rates in solutions, effect of dielectric constant and ionic strength, cage effect, Bronsted-Bjerrum equation.

**Module 3** **Catalysis-I** **14 hrs**

Kinetics and mechanisms of homogeneous and heterogeneous catalysis, autocatalytic reactions, catalytic promoters and catalytic inhibitors, acid base catalysis, acid functions, Enzyme catalysis: influence of substrate concentration :single substrate: Michaelis-Menten equation, and double substrate reactions, kinetics of inhibition, effects of pH, temperature, on enzyme catalyzed reactions and its applications,

**Module 4** **Catalysis-II** **10 hrs**

Kinetics of surface catalysed reaction: Langmuir Hinshelwood and Rideal model, catalysis by metals and semiconductors, Electronic factors of catalysis by metals and semiconductors, Charge transfer theory of catalysis, Electronic theory of catalysis by metals, Ammonia synthesis and oxidation of CO.

**References/compulsory reading**

1. *Chemical Kinetic Methods: Principles of Relaxation Techniques and applications*, C. Kalidas, New Age International
2. *Chemical Kinetics*, K.J. Laidler, Pearson Education
3. *Fundamentals of Photochemistry*, K.K. Rohatgi - Mukkerjee, Wiley Eastern Ltd.
4. *Introduction to Molecular Dynamics and Chemical Kinetics* G.D. Billing and K.V. Mikkelsen, John Wiley
5. *Kinetics and Mechanisms of Chemical Transformations*, J. Rajaram and J.C. Kuriacose, Macmillan
6. *Molecular Reaction Dynamics and Chemical Reactivity*, R.D. Levine, R.B. Bernstein Oxford
7. *Reaction Kinetics*, M.J. Pilling and P.W. Seakins, Oxford Univ. Press
8. *The Principles of Electrochemistry*, D.R. Crow, Chapman and Hall
9. *Heterogeneous Catalysis* by Thomas & Thomas
10. *Metal Oxides in Heterogeneous Catalysis*, Jacques C. Vedrine, Elsevier
11. *Modern Heterogeneous Catalysis: An Introduction*, Rutger A. van Santen, Wiley-VCH

**Supplementary and suggested reading**

1. *Physics and Chemistry of Surfaces* by Adamson
2. *Kinetics and Mechanisms*, J. W. Moore & R.G. Pearson, John Wiley & Sons,
3. *The theory of Rate Process*, S. Glasstone, K. J. Laidler and H. Eyring, McGraw Hill.
4. *Physical Chemistry*, R. A. Albert and R. J. Silby,, Wiley Eastern
5. *Heterogeneous Catalysis Fundamentals and Applications*, 1st Edition, Julian R.H. Ross, Elsevier
6. *Physical Chemistry*, Atkins, P.W., W.H. Freeman ,Oxford University

## MSCHE03C12: Physical Chemistry Practical

### Aim and Objectives

To make the students

1. Expertise in the applied concepts of kinetics, electrochemistry, thermodynamics, phase equilibrium, adsorption, etc.
2. Draw structures and graph using softwares and prepare reports

### Learning Outcome

Students will be able to:

1. Interpret data from an experiment, including the construction of appropriate graphs and the evaluation of errors.
2. Construct the Freundlich and Langmuir isotherms for adsorption of acetic/oxalic acid on active charcoal/ alumina and determine the concentration of acetic/ oxalic acid
3. Determine the rate constant, Arrhenius parameters, rate constant and concentration using kinetics
4. Construct the phase diagram and determine the composition of an unknown mixture
5. Construct the ternary phase diagram of acetic acid chloroform-water system and out the procedure in an unfamiliar situation to find out the composition of given homogeneous mixture.
6. Construct the tie-line in the ternary phase diagram of acetic acid chloroform-water system
7. Determine distribution coefficient using distribution law.
8. Determine  $K_f$  of solid solvent, molar mass of non-volatile solute, mass of solvent and composition of given solution
9. Determine surface tension and parachor of liquids.
10. Ascertain the relationship between surface tension with concentration of a liquid and use this to find out the composition of given homogeneous mixture.
11. Determine the concentration of given strong acid/alkali.
12. Determine the heat of ionisation of acetic acid.
13. Interpret data from an experiment, including the determine the strength of strong/ weak acids by conductometric titration
14. Verify Onsager equation and Kohlraush's law conductometrically .
15. Determine the activity and activity coefficient of electrolyte.
16. Determine the concentration of a solution potentiometrically or pH metrically.
17. Employ spectrophotometry in determining unknown concentration.
18. Determine the viscosity of liquid mixtures and use this in determining the concentration of a component in a mixture.
19. Determine the concentration of a liquid mixture using a refractometer.
20. Determine the unknown concentration of a given glucose solution.

### Module 1

#### Distribution methods

54 hrs

Distribution law: Partition of iodine between water and carbon tetrachloride, Equilibrium constant of simple reaction, concentration of unknown KI, partition studies, determination of equilibrium constant, hydrolysis constant, association studies, Solid and liquid equilibria:

### Module 2

#### Phase equilibria studies

54 hrs

Construction of phase diagram of simple eutectics, systems with congruent melting points and solid solutions, determination of composition of unknown mixtures, analytical and synthetic methods for the determination of solubilities and heat of solution.

Partially miscible liquids: Critical solution temperature, influence of impurities on the miscibility temperature, determination of composition of unknown mixtures, completely miscible liquid systems: Construction of phase diagrams of two component liquid systems, Zeotropic and azeotropic. Three

component systems: With one pair of partially miscible liquids, construction of phase diagrams and tie lines, compositions of homogenous mixtures, heat of solution from solubility data, analytical and graphical method.

**Module 3                      Molecular weight determination & refractometry                      54 hrs**

Molecular Weight Determination, Rast and transition temperature method, molecular weight of a solid using a solid solvent by cooling curve method, molecular weight determination by study of depression in transition temperature, cryoscopic study,

Refractometry: Determination of molar refractions of pure liquids, determination of composition of mixtures.

Viscosity: Determination of viscosity of pure liquids, composition of binary liquid mixtures determination of molecular weight of a polymer.

**Module 4                      Electrochemical and spectrochemical studies                      54 hrs**

Potentiometry: Electrode potentials of Zn and Ag electrodes, determination of standard potentials, determination of mean activity co-efficient of an electrolyte at different molalities by EMF method, dissociation constant measurement, determination of strength of a given solution, potentiometric titration.

- 1 Flame photometry: quantitative determination of Na<sup>+</sup>, K<sup>+</sup>, Li<sup>+</sup> and Ca<sup>2+</sup> ions
- 2 Polarography: determination of number of components and concentration (Cd<sup>2+</sup>, Zn<sup>2+</sup>, Pb<sup>2+</sup>, Cu<sup>2+</sup>, etc.)
- 3 Kinetics of salt effect
- 4 Determination of Transport number
- 5 Conductance study of saponification reaction
- 6 Potentiometry: determination of stability constant of Cu<sup>2+</sup> and ethelenediamine
- 7 UV-Vis. Spectrophotometer: determination of the order of a reaction
- 8 Colorimetry: quantitative determination of the components of a binary mixture
- 9 Computer applications in chemistry
- a) Chem draw/ ISIS sketches for reaction and mechanism (minimum 3 Nos)
- b) C<sup>++</sup> programming for the calculation of thermodynamic parameters

**References:**

1. *A Text Book of Quantitative Inorganic Analysis*, A.I. Vogel, Pearson Education
2. *Experimental Inorganic Chemistry*, W.G. Palmer, Cambridge University Press.
3. *Experimental Physical Chemistry*, D.P. Shoemaker and C.W. Garland, McGraw-Hill.
4. *Experimental Physical Chemistry*, F. Daniels and J.H. Mathews, Longman.
5. *Experimental Physical Chemistry*, V.d. Ahuwale and parul, New age International.
6. *Instrumental Methods of Analysis*, H.H. Willard, L.L. Merritt and J.A. Dean, AEWt Press.

**Supplementary/ Suggested reading**

1. *Practical Physical Chemistry* A M James, J A Churchil
2. *Practical Physical Chemistry*, A. Finlay and J. Akitchener, Longman
3. *Practical Physical Chemistry*, D.M. James and F.E. Prichard, Longman

**MSCHE03E08: Analytical Chemistry**

**Aim and Objectives**

1. The primary objective of this course is to acquire basic concepts, principles, and techniques of modern analytical chemistry that would empower students with an analytical mind set and the abilities to solve diverse analytical problems in an efficient and quantitative way that conveys the importance of accuracy and precision of the analytical results.

2. To know about the latest characterisation techniques and instrumentation details of sophisticated instruments.

### **Learning Outcomes**

On successful completion of this course, students will be able:

1. To develop an understanding of the range and uses of analytical methods in chemistry.
3. To establish an appreciation of the role of chemistry in quantitative analysis
4. To develop an understanding of the broad role of the chemist in measurement and problem solving for analytical tasks.
5. To provide an understanding of instrumental methods employed for elemental and compound analysis.
6. To provide experience in modern scientific methods and instruments employed in analytical chemistry and material science.
7. To develop some understanding of the professional and safety responsibilities residing in working on chemical analysis.

### **Module 1 Introduction to analytical methods-I 18 hrs**

Introduction to analytical and instrumental methods, Classification of analytical techniques, nature and origin of errors, accuracy and precision, statistical evaluation of data, tests of significance, Students 't' test, 'F' test, significant figures and computation rules, Types of analysis based on sample size : macro, meso, micro, sub-micro and ultra-micro estimations, nano level detections. Precipitation phenomena, organic precipitants in inorganic analysis, extraction of metal ions, nature and types of extractants and its applications, chelometric titration, masking and de masking techniques, industrial applications of masking. Separation techniques: Solvent extraction, batch and continuous extractions, countercurrent distribution, extraction of metal ions, nature and types of extractants and its applications.

### **Module 2 Introduction to analytical methods-II 18 hrs**

Introduction to chromatography, classification of chromatographic methods, theory, techniques and applications of Paper chromatography, Column chromatography, Thin layer chromatography (TLC), high performance liquid chromatography (HPLC), Gas chromatography (GC). Radio analytical methods: Introduction, principle and application of neutron activation analysis (NAA), isotope dilution analysis and radiometric titrations. Electro analytical methods: Principles and applications of Voltammetry, Cyclic voltammetry (CV), Polarography, Stripping voltammetry, Conductometry, Amperometry, Potentiometry and Electrogravimetry.

### **Module 3 Instrumental methods of analysis-I 18 hrs**

Introduction to instrumentation, method of samplings, data analysis and applications to chemistry of the followings, Attenuated Total Reflection Spectroscopy, X-Ray Fluorescence, Electronic Spectroscopy for Chemical Analysis (X-ray Photo Electron Spectroscopy), UV-Photo Electron Spectroscopy, Ion Scattering Spectroscopy, Secondary Ion Mass Spectroscopy, Auger Electron Spectroscopy, Principles, general instrumentation and applications of Scanning Electron Microscopy, Scanning Tunneling Electron Microscopy, Atomic Absorption Spectroscopy and X-ray crystallography.

### **Module 4 Instrumental methods of analysis-II 18 hrs**

Principles, instrumentation and applications of thermogravimetry (TGA-DTA), Differential Scanning Calorimetry, Dynamic Mechanical Analyzer, Dynamic Chemical Analyzer, Direct injection

enthalpymetry and thermometric titrimetry, Principles, instrumentation and applications of Fluorimetry, Phosphorimetry, Flame photometry, Nephelometry and Turbidimetry, Instrumentations of NMR, IR, UV-Visible and Mass spectrometry

**References:**

1. *Fundamentals of Analytical Chemistry*, Skoog, West, Holler, Croach, Thomson Brooks/Cole
2. *Instrumental methods of chemical analysis*, Willard, Dean and Merrit, Affiliated East West Press
3. *Modern analytical chemistry*, Harvey, Mc Graw Hill
4. *Organic Analytical Chemistry*, Jagmohan, Narosa Publications
5. *Principles and practice of Analytical Chemistry*, F.W. Fifield and D. Kealeg, Blackwell publications

**Supplementary/ Suggested reading**

1. *Principles of quantitative chemical analysis*, de Levine, Mc Graw Hill
2. *Vogel's Qualiitative Inorganic Analysis*, Pearson Education
3. *Vogel's Quantitative chemical analysis*, Pearson Education

**MSCHE03E09: Polymer chemistry**

**Aims and Objectives:**

1. To describe general structure of polymers
2. To account for the concept of molecular weight of polymers.
3. To understand various types of polymerisation their kinetic and thermodynamic considerations.
4. To introduce the concepts of polymers in solution and in solid state
5. To correlate the properties and structure of polymers
6. Impart awareness on the types of polymers and their industrial applications

**Learning Outcomes:**

Upon successful completion of this course, students will be able to:

1. To acquire theoretical knowledge and understanding of fundamental concepts, principles and processes of main branches of polymer science
2. To understand the concepts of molecular weight and the methods of determination.
3. Describe how polymer morphology affects a polymer's overall properties and behavior
4. To have awareness on the methods of synthesis, kinetics and thermodynamics of various polymerisation processes.
5. Understand the significance and industrial relevance of polymers

**Module 1      Classification, structure, and properties of polymers      24 hrs**

Basic Concepts-Classification, nomenclature, molecular weight and distribution, glass transition, morphology, viscosity vs. molecular weight and mechanical property vs. molecular weight relationships, Chain structure and configuration. Methods of determination of molecular weight, distribution, size and shape of polymers, Intrinsic viscosity, Mark-Houwink relationship, Thermodynamics of polymer solutions, self-diffusion, reptation, Rouse-Bueche theory and de Gennes reptation model.

**Module 2      Polymerization techniques      24 hrs**

Polymerization techniques: condensation polymerization, kinetic and thermodynamic considerations, molecular weight distribution, chain polymerization: effect of substituents, factors affecting polymerization, methods of polymerization: living polymerization, transfer- radical-polymerization.



Cationic chain polymerization, kinetics and energetics, anionic polymerization: chain copolymerization, determination of composition, ring-opening polymerization, Ziegler-Natta catalyst, control of stereochemistry of polyolefins and polycyclo-olefins. Metathesis polymerization: mechanisms, synthesis of polyacetylenes, synthesis block, graft copolymers,

**Module 3 Characterization techniques of polymers 12 hrs**

Characterization techniques of polymers: thermal, mechanical and structural characterizations. Glass transition temperature and its methods of determination Mechanical properties of polymers and methods of determination

**Module 4 Speciality polymers & polymer composites 12 hrs**

Speciality polymers: fire retardant polymers, liquid crystalline polymers, biodegradable polymers, high temperature polymers, optic fibers. Polymer composites: fibre composites, reinforcing mechanisms, failure mechanism in composites, composite fabrication techniques, applications

**References**

1. S.R. Sandler, W. Karo, *Polymer Synthesis, Vol.2, Academic Press, 1993.*
2. S.R. Sandler, W. Karo, *Polymer Synthesis, Vol.3, Academic Press, 1998.*
3. D. C. Blackley, *Polymer Latices, Vol.1, 2 & 3, 2nd Edn., Springer, 1997.*
4. W.C. Wake, *Analysis of Rubbers and Rubber like Polymers, 2nd Edn, Wiley-Interscience, 1969*
5. F. W. Billmeyer, *Textbook of Polymer Science, 3rd Edition, John Wiley, 1994.*
6. Gowariker et al, *Polymer Science. Wiley Eastern, 1990.*

**Supplementary/Suggested Reading**

1. *Introduction to Physical Polymer Science L. H. Sperling, Wiley- Interscience*
2. *J. Ivin and J. C. Mol, Olefin Metathesis, 2nd edition, Academic Press, 1996.*
3. *Principles of Polymer Chemistry, P. J. Flory, Cornell University Press, 1953.*
4. *Principles of Polymerization G. Odian, , Third edition, Wiley-Interscience.*

**MSCHE03E10: Biochemistry**

**Aim and Objectives**

1. Considered as one of the molecular sciences, biochemistry is a branch of both chemistry and biology; The main goal of biochemistry is to understand the structure and behavior of biomolecules.
2. To introduce the role of biochemistry in our daily life.

**Learning outcome.**

1. Learners will recognize the different biomolecules and their structure.
2. Understand the function of enzymes as catalysts in biochemical reactions.
3. How the study of various aspects of health and disease has opened up new areas of biochemistry.
4. Understand the scope of applications of biochemistry/Biomaterials in Medical field.
5. Develop an interest in research areas of Biochemistry.

**Module 1 Chemistry of biomolecules 18 hrs**

Cell structure: Chemistry of biomolecules, basic aspects of structure and classification of carbohydrates, lipids, aminoacids, proteins and nucleic acids. Supramolecular assemblies, biomembranes, lipo and glycoproteins.

**Module 2 Biocatalysis 18 hrs**

Biocatalysis, concept of enzyme catalysis, role of vitamins and metals as cofactors, enzyme kinetics, Michaelis-Menten equation, inhibition of enzyme action, regulatory aspects, Metabolism: Overview and important relationships between-glycolysis, TCA cycle, HMP shunt, oxidation of fatty acids, amino acids and urea cycle. Flow of genetic information, nature of genetic code, replication of DNA, transcription and translation, regulation of gene expression.

**Module 3 Bioactive polymers and ceramics 18 hrs**

Bioactive and biodegradable polymers: bioactive ceramics. Biocompatibility, toxicity, cytotoxicity, hypersensitivity, Protein interaction with synthetic materials. Immunological responses to biomaterials, blood compatibility, platelet adhesion and aggregation, coagulation, Assessment of blood: compatibility, sterility and infection.

**Module 4 Biomaterials 18 hrs**

Interactions of bacteria with biomaterials, methods for sterilization, assessment of sterility, Cardiovascular applications: grafts, catheters, stents, valves, embolic agents, orthopedic applications- joint prostheses, fracture fixation devices, ophthalmologic applications, contact lenses, corneal implants, Dental materials and implants

**References/compulsory reading**

1. *Biochemistry*, Christopher K. Mathews and K. E. Von Holder, Benjamin/Cummings.
2. *Biochemistry*, Lubert Stryer, W. H. Freeman and Company, 4th edition.
3. *Biomaterial Science- An introduction to Materials in Medicine*, B.D. Ratner, A.S. Hoffman, F.J. Schoen and J.E. Lemons, Academic press
4. *Biomaterials: Principles and applications*, J.B. Park, J.D. Bronzino, CRC Press
5. *Design Engineering of Biomaterials for Medical Devices*, David Hill, John Wiley and Sons
6. *Principles of Biochemistry* Albert L. Lehninger, David L. Nelson, Michael M. Cox., CBS Publishers and Distributors.

**Supplementary/Suggested Reading**

1. *Biochemistry (2 Volume Set): The Chemical Reactions of Living Cells* Metzler, David E.. Elsevier, 2003.
2. *Biochemistry: a short course*. Tymoczko, John L., Jeremy M. Berg, and Lubert Stryer. Biochemistry: a short course. Macmillan, 2011.
3. *Biochemistry*, Garrett, Reginald, and Charles Grisham.. Nelson Education, 2012.
4. *Fundamentals of biochemistry* Voet, Donald, Judith G. Voet, and Charlotte W. Pratt. "Fundamentals of biochemistry New York: John Wiley & Sons 2008

**MSCHE03E11: Study Tour Report**

Students will have to visit a Research Institute of National repute to have an idea about the current research activities. The report of the same may be submitted to the head of the department for valuation

## FOURTH SEMESTER

### MSCHE04C13: Research Project

Each student shall carry out a project work in any branches of Chemistry/ Material Science for a period of not more than six months. The project can be carried out in a research institute/industry of national repute with guidance from experts there.

### MSCHE04C14: Comprehensive Viva

A Comprehensive viva is conducted at the end of the Semester by external experts from other University/research institutions suggested by the Head of the Department and approved by the Vice Chancellor.

### MSCHE04E12: Inorganic and Nano Materials

#### Aims and Objectives:

1. To understand the basic concepts of inorganic materials and their classifications
2. To impart knowledge on the application and industrial relevance of inorganic materials like alloys and metal oxides
3. To introduce the concepts of bonding in different metal oxides, borides, nitrides, carbides, borides etc
4. Introducing the concept of metallurgy
5. To introduce the foundational knowledge of Nanoscience and technology in a broad aspect including background, concepts and misconceptions.
6. Explain the effect of quantum confinement on the electronic structure on physical chemical and mechanical properties.
7. To introduce various synthesis methods and make them able to choose an appropriate one depending upon the desired size and morphology
8. To impart awareness on various characterization methods based on the phase morphological and optical characteristics of different nanomaterials

#### Learning Outcomes:

Upon successful completion of this course, students will be able to:

1. Have a fundamental knowledge on the various aspects of inorganics and nanostructures
2. Understand the industrial relevance of inorganic materials
3. Structural properties of various oxides borides silicides etc
4. Understand deeply the metallurgical processes for the extraction of various metals
5. Have a board outline on the history and emergence of Nanoscience and Technology
6. Acquire knowledge of various nanomaterials in terms of quantum confinement and the impact of each type in their properties
7. Understand the concepts applicable during the synthesis and formation of nano-materials like top down and bottom up approaches, grain boundaries aggregation etc
8. Synthesize Nanomaterials of different size and morphology by choosing appropriate methods.
9. Understand various characterization techniques for the nanostructures

#### Module 1

#### Inorganic materials-I

18 hrs

Metals and alloys relevant to aerospace applications, Chemistry of Titanium and its alloys, study of ilmenite, Extraction of titanium, its alloys and Shape memory alloys, their applications, Structure and technological importance of silicates, cement and ceramics, chemistry of metallocycles, cages and clusters of elements, cryptands and calixerenes, biological significances, Structural variety properties

and implications of borides, carbides, silicides, nitrides, phosphides, oxides and sulfides of transition elements, multiple bonds and cluster variety of transition metals, higher boranes, carboranes and metalloboranes.

**Module 2 Inorganic materials-II 18 hrs**

Methods of reduction of oxide ores, Ellingham diagram, chemical and electrolytic reductions, reduction potentials, Latimer and Frost diagrams, effect of complexation on potential. Lanthanide and actinides: electronic structure, oxidation states, extraction and separation of lanthan

**Module 3 Nanomaterials-I 18 hrs**

Nanoscience an introduction, nanomaterials and nanocomposites, surface energy, thermodynamics, phase transformations. Structure of nanomaterials:- tubes, fibers, wires, bricks and building blocks. Synthesis:- condensation, vapour synthesis, laser ablation, microwave plasma and flame aerosol processes. Nanostructure formation: lithography, self-assembly, molecular synthesis, crystal growth and polymerization, Properties of nanomaterials:- magnetic, optical, electrical and mechanical properties, superparamagnetic materials, transparent matrices, photochromic and electrochromic materials.

**Module 4 Nanomaterials-II 18 hrs**

Measurement of nanostructure:- specific surface area, X-ray and electron diffraction, electron microscopy, STEM, NanoCAD, Material study: nanocomposites, consumer goods, 'smart materials', Applications to various fields: optics, telecommunication, electronics, digital technology and environment, Biomedical applications: diagnosis, protean engineering, mapping of genes, drug delivery, biomimetics, quantum dots.

**References**

1. *Nanotechnology: basic science and emerging technologies* – Mick Wilson, Kamali Kannangara, Geoff Smith, Michelle Simmons, Burkhard Raguse, Overseas Press (2005)
2. *Nanocomposite science and technology*, Pulickel M.Ajayan, Linda S.Schadler, Paul V.Braun, Wiley-VCH Verlag, Weiheim (2003).
3. *Amorphous and Nanocrystalline Materials: Preparation , Properties, and Applications*, A.Inoue, K.Hashimoto (Eds.,) (2000)
4. *Understanding Nanotechnology*, Scientific American, editors at Scientific American, Warner Books (2002) Anx.46 B - M Sc Nanosci & tech (CBCS) 2008-09.
5. *Introduction to Nanotechnology* by Charles P. Poole, Frank J. Owens, WileyInterscience (2003).
6. *Nanotechnology: A Gentle Introduction to the Next Big Idea*, Mark A. Ratner, Daniel Ratner, Mark Ratne, Prentice Hall PTR; 1st edition (2002)

**Suggested/Supplementary Reading**

1. *Nanocomposites*, diwan, Bharadwaj, Pentagon
2. *Nanotechnology*, W. Kannangara, Smith, Chapman and hall
3. *Nanomaterials*, bandyopadhyay, New age international
4. *Nnaomaterials*, D. Vollath, Wiley-Vch
5. *Nanochemistry*, G.A. Ozin, A.C. Arsenault, RSC

**MSCHE04E13: Ceramics, Composites and inorganic polymers**

**Aims and Objectives:**

1. To introduce the different types of ceramics and composite materials, their properties and applications.
2. To introduce the special characteristics and fabrication methods of different classes of



6. *Composite Materials: Engineering and Science - F. L. Matthews and R. D. Rawlings, Chapman & Hall .*
7. *Advanced Composite Manufacturing - Gutowski, Wiley.*
8. *Inorganic polymers, Mark JE, Allcock HR, West R. Oxford University Press, New York*
9. *Inorganic and organometallic polymers, Chandrasekhar V . Springer.*

#### **Supplementary and suggested readings**

1. *Polymer composites, M.C. Gupta and A.P. Gupta, New Age International*
2. *Introduction to polymers, Young and Lowell, Viva Publications*
3. *Advanced Polymer Chemistry, Chanda, Manas, CRC.*
4. *Contemporary polymer chemistry, Allcock, Lampe and Marle, Pearson education*
5. *Ceramic Materials for Electronics, R. C. Buchanan (ed.), Marcel Dekker.*
6. *Introduction to the Principles of Ceramic Processing, J. S. Read, Wiley-Interscience.*

### **MSCHE04O01: Contemporary Chemistry**

#### **Aims and Objectives**

1. To learn the different types of materials in chemistry
2. To study the nanomaterials chemistry
3. To learn about the chemistry of everyday use to human
4. To make an aware of the environmental aspects of chemistry
5. To study the various components of medicine and food

#### **Learning Outcomes**

1. The learner will be able to explain the different types of nanoparticles and their applications to various fields
2. The learner can explain the preparation, properties and applications of useful polymers
3. The student can have the idea of preparation and chemistry of soaps and detergents
4. The student will learn chemical components of different types of cosmetics, sensitizers, handwash, talcum powder and fresheners
5. The learner can explain the cause, effect and control measures of air, water and soil pollution
6. The student can describe the properties and structure of amino acids, peptides and proteins, enzymes and drugs

|                 |                               |               |
|-----------------|-------------------------------|---------------|
| <b>Module 1</b> | <b>Chemistry of Materials</b> | <b>18 hrs</b> |
|-----------------|-------------------------------|---------------|

Different types of nanoparticles. applications of nanoparticles in medicine and electronics, Quantum dots, Preparation, properties and applications of polyurethane, polythene, polyvinyl chloride and polyamides, synthetic rubbers and conducting polymers

|                 |                              |               |
|-----------------|------------------------------|---------------|
| <b>Module 2</b> | <b>Chemistry of Everyday</b> | <b>18 hrs</b> |
|-----------------|------------------------------|---------------|

Preparation and chemistry of soaps and detergents, General chemical components of different types of cosmetics, sensitizers, handwash, talcum powder and fresheners, Food additives, food adulteration, carbohydrates, oils and fats, Types of fertilizers, Bio-fertilizers

|                 |                                     |               |
|-----------------|-------------------------------------|---------------|
| <b>Module 3</b> | <b>Chemistry of the Environment</b> | <b>18 hrs</b> |
|-----------------|-------------------------------------|---------------|

Issues and possible solutions of Environmental ethics, Cause, effect and control measures of air, water and soil pollution, greenhouse effect, laboratory safety precautions, Principles of green chemistry, Toxicology of nanoparticles, Nuclear waste and its impact on the environment

**Module 4****Chemistry of Life****18 hrs**

Classification, properties and structure of amino acids, peptides and proteins, Components of Nucleic acids, Nucleosides and nucleotides, DNA, RNA and their biological functions, Enzymes, Coenzymes and cofactors and their role in biological reactions, Classification of drugs - Analgesics, Antipyretics, Antihistamines, Antacids, Antibiotics and Antifertility drugs

**References**

1. *Nanoscale Materials in Chemistry*, K.J. Klabunde, Wiley.
2. *Chemistry in Daily Life*, Singh, K., Prentice Hall of India
3. *Chemistry of Pesticides*, K.H. Buchel, John Wiley & Sons, New York, 1983
4. *Polymer Science*, V.R. Gowariker; N.V. Viswanathan and J. Sreedhar, New Age
5. *Text Book of Environmental Studies for undergraduate Courses*, Bharucha Erach, University Press
6. *Environmental Chemistry*, Day A.K, Wiley Eastern Ltd
7. *Nuclear Chemistry*, U.N. Dash, Sultan Chand and Sons
8. *Biochemistry*, Berg, J.M., Tymoczko, J.L. & Stryer, L., W.H. Freeman
9. *Chemistry of Natural Products*, Bhat S.V., Nagasampagi, B.A. Sivakumar M., Narosa

**Supplementary/Suggested Readings**

1. *Chemistry for Changing Times*, J.W. Hill; T.W. McCreary and D.K. Kolb, Prentice Hall
2. *Environmental Encyclopedia*, Cunningham, W.P. Cooper, T.H. Gorhani, E. Hepworth, M.T. Jaico Publ. House.
3. *Medicinal Chemistry*, D. Sriram and P. Yogeeswari, Pearson

**Model Question Paper**  
First Semester M.Sc Degree (CCSS) Examination  
**CHEMISTRY**  
**MSCHE01C02 - Electro Chemistry, Electrode and Phase Equilibria**  
(2020 Admission onwards)

Time : 3 hours

Max: Marks : 60

**SECTION A**

*Answer **any five** questions (Each question carries 3 marks)*

1. Briefly describe the concept of triple ions.
2. Estimate the mean activity coefficient of 0.005M Na<sub>2</sub>SO<sub>4</sub> at 25°C (A= 0.509)
3. Define ionic mobility. How is it related to specific conductance.
4. What is asymmetry effect?
5. Give one example of abnormal ion conductance.
6. What is Debye-Huckel limiting law. Explain its significance.

*(5 x 3 = 15)*

**SECTION B**

*Answer **any three** questions (Each question carries 5 marks)*

7. Apply phase rule for a two component system with a partially miscible solid phases and discuss.
8. "Gibbs energy of a substance has close connection to its phase diagram". Explain.
9. Explain 'peritectic systems' of partially miscible solid phase with an example.
10. Deduce an expression for the thickness of ion atmosphere using Debye-Huckel theory.
11. How do you verify Debye Huckel limiting law experimentally. Discuss.

*(3 X 5 = 15)*



### SECTION C

Answer **any three** questions (Each question carries 10 marks)

12. A) Derive Butler-Volmer equation for simple electron transfer reactions. B) What is Wein effect?
13. A) Deduce Debye-Huckel Onsager equation . Discuss its validity. B) Explain the physical significance of activity.
14. A) Explain the theories of overvoltage. B) What is liquid junction potential? How is it eliminated?
15. A) Derive the phase rule. B) Explain the phase diagram of a system with transition point.
16. A) What are the conditions required to exist equilibrium between phases?  
(B) With the help of phase diagram discuss double salt formation

(3 x 10 = 30)

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**Model Question Paper**  
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*(5 x 3 = 15)*

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8. "Gibbs energy of a substance has close connection to its phase diagram". Explain.
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10. Deduce an expression for the thickness of ion atmosphere using Debye-Huckel theory.
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14. A) Explain the theories of overvoltage. B) What is liquid junction potential? How is it eliminated?
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