

**Dr. AMBEDKAR GOVERNMENT ARTS COLLEGE (AUTONOMOUS)**  
**CHENNAI – 600039.**

**DEPARTMENT OF CHEMISTRY**

**Date : 12. 06. 2019, Wednesday**

**Time : 12.15 p.m.**

**AGENDA – M.Sc. CHEMISTRY**

- To discuss the course content of the existing syllabus
- To suggest suitable modifications and
- To consider and approve the modified syllabus

C. Srinivasa  
**Chairman** 12/6/19

University Nominee

- Mr.A.Gopalakrishnan

- A. Gan

Subject Expert 1

- Dr.V.Sivamurugan

- V. Sivamurugan

Subject Expert 2

- Dr.S.Balasubramanian

- S. Balasubramanian 12/6/19

Industrial Nominee

- Mr.G.Chandrasekar

- G. Chandrasekar

Alumni

- Mr.R.Giridharan

- R. Giridharan

Dept Staff Members

- Dr.R.Ravichandran

-

- Dr.R.Karthikeyan

- R. Karthikeyan 12/6/19

- Dr.S.Manivannan

- S. Manivannan 12/6/19

- Mr.K.Chandrasekaran

- K. Chandrasekaran 12/6/19

- Mrs.T.Gayathri

- T. Gayathri 12/6/19

- Dr.P.Krishnamurthy

- P. Krishnamurthy 12/6/19

- Mrs.S.Ananthi

- S. Ananthi 12/6/19

- Dr.T.K.Arumugam

- T. K. Arumugam 12/6/19

- Mrs.RevathySelvaraj

- Revathy Selvaraj 12/6/19

- Dr.G.Ramesh

- G. Ramesh 12/6/19

- Dr.G.Ramachandran

- G. Ramachandran 12/6/19

- Dr.S.Shanmugasundari

- S. Shanmugasundari 12/6/19

- Dr.S.Vidya

- S. Vidya 12/6/19

- Dr.L.Lakshmi

- L. Lakshmi 12/06/2019

**Dr. AMBEDKAR GOVERNMENT ARTS COLLEGE (AUTONOMOUS)  
CHENNAI – 600039.**

**DEPARTMENT OF CHEMISTRY**

**Minutes of the Meeting of Board of Studies in M.Sc., CHEMISTRY**

**Date :** 12. 06. 2019, Wednesday

**Time :** 12.15 p.m.

- The Curriculum was revised based guidelines laid down by Tamilnadu State Council for Higher Education (TANSCH)
- The members of the Board discussed the course content in details and incorporated necessary changes.

**The following resolutions were adopted in the meeting**

RESOLVED that the draft syllabi proposed for M.Sc., Chemistry by the Department of Chemistry were discussed and approved with the following changes and decided to implement the same for the students admitted from the academic year 2019-2020.

- For Elective subjects Environmental Chemistry, Bioinorganic Chemistry, Chemistry of Biomolecules, Modern synthetic strategies and Green Chemistry and Material chemistry were introduced.
- For Extra disciplinary elective Research Methodology and Biochemistry were introduced.
- Practical Examinations are to be conducted at the end of Even semester as per the regulations of University of Madras.
- Soft skills subjects are as per University of madras regulations.

*C. Srinivasan*  
12/6/19  
**CHAIRMAN**

**Dr. AMBEDKAR GOVERNMENT ARTS COLLEGE (AUTONOMOUS)  
CHENNAI – 600039.**

**DEPARTMENT OF CHEMISTRY**

**Minutes of the Meeting of Board of Studies in M.Sc., CHEMISTRY**

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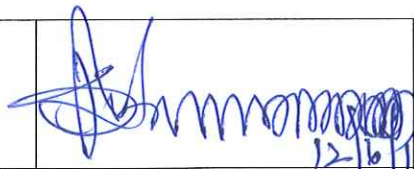
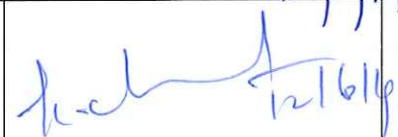
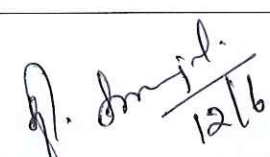
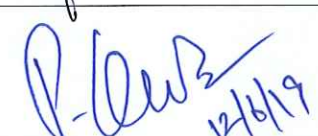
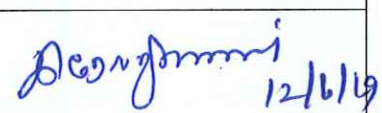
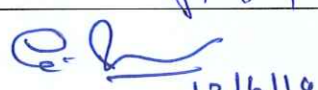
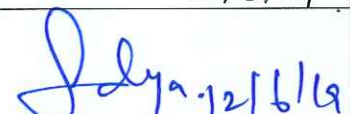
**MEMBERS PRESENT**

| S.No | NAME                        | DESIGNATION                                                                                | MEMBERSHIP            | SIGNATURE                                                                             |
|------|-----------------------------|--------------------------------------------------------------------------------------------|-----------------------|---------------------------------------------------------------------------------------|
| 1    | <b>Dr.C.Srinivasan</b>      | Assistant Professor of Chemistry and Head i/c                                              | CHAIRMAN              |    |
| 2    | <b>Mr.A.Gopalakrishnan</b>  | Assistant Professor of Chemistry,<br>D.G Vaishnav College,<br>Arumbakkam,<br>Chennai-106.  | UNIVERSITY<br>NOMINEE |    |
| 3    | <b>Dr.V.Sivamurugan</b>     | Assistant Professor of Chemistry<br>Pachaiappa's College,<br>Chennai-600 030               | SUBJECT<br>EXPERT -1  |  |
| 4    | <b>Dr.S.Balasubramanian</b> | Assistant Professor of Chemistry<br>Presidency<br>College, Chennai-600 005                 | SUBJECT<br>EXPERT -2  |  |
| 5    | <b>Mr.G.Chandrasekar</b>    | General Manager,<br>R & D / QA<br>Raj Petro Specialties<br>Pvt Limited<br>Manali, Chennai. | INDUSTRY<br>NOMINEE   |  |
| 6    | <b>Mr. Giridharan</b>       | M.Sc. Chemistry<br>(2012-2014 Batch)                                                       | ALUMNI                |  |

**FACULTY MEMBERS OF THE CHEMISTRY DEPARTMENT**

|   |                           |                     |        |                                                                                       |
|---|---------------------------|---------------------|--------|---------------------------------------------------------------------------------------|
| 7 | <b>Dr. R.Ravichandran</b> | Assistant Professor | MEMBER |                                                                                       |
| 8 | <b>Dr. R. Karthikeyan</b> | Assistant Professor | MEMBER |  |



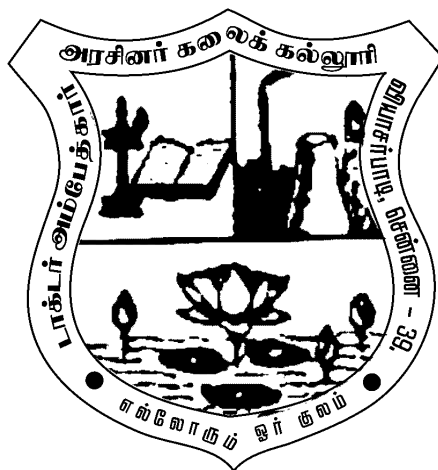
|    |                             |                     |        |                                                                                                     |
|----|-----------------------------|---------------------|--------|-----------------------------------------------------------------------------------------------------|
| 9  | <b>Dr.S.Manivannan</b>      | Assistant Professor | MEMBER | <br>12/6/19.     |
| 10 | <b>Mr.K.Chandrasekaran</b>  | Assistant Professor | MEMBER | <br>12/6/19      |
| 11 | <b>Mrs.T.Gayathri</b>       | Assistant Professor | MEMBER | <br>12/6         |
| 12 | <b>Dr.P.Krishnamoorthy</b>  | Assistant Professor | MEMBER | <br>12/6/19      |
| 13 | <b>Mrs.S.Ananthi</b>        | Assistant Professor | MEMBER | <br>12/6/19      |
| 14 | <b>Dr.T.K.Arumugam</b>      | Assistant Professor | MEMBER | <br>12/6/19      |
| 15 | <b>Mrs.RevathySelvaraj</b>  | Assistant Professor | MEMBER | <br>12/6/19    |
| 16 | <b>Dr.G.Ramesh</b>          | Assistant Professor | MEMBER | <br>12/6/19    |
| 17 | <b>Dr.G.Ramachandran</b>    | Assistant Professor | MEMBER | <br>12/6/19    |
| 18 | <b>Dr.S.Shanmugasundari</b> | Assistant Professor | MEMBER | <br>12/6/19    |
| 19 | <b>Dr.S.Vidya</b>           | Assistant Professor | MEMBER | <br>12/6/19    |
| 20 | <b>Dr.L.Lakshmi</b>         | Assistant Professor | MEMBER | <br>12/06/2019 |

**DR.AMBEDKAR GOVERNMENT ARTS COLLEGE**

**( AUTONOMOUS)**

**VYASARPADI, CHENNAI – 600 039.**

**Accredited by NAAC at level B**



**Syllabus for M.Sc. Chemistry**

**Under CBCS**

**(Under Semester system with credits)**

**Effective from the academic year 2019-2020**

**POST GRADUATE AND RESEARCH DEPARTMENT OF CHEMISTRY**

**DR. AMBEDKAR GOVERNMENT ART COLLEGE**  
**(AUTONOMOUS)**  
**VYSARPADI, CHENNAI – 600 039.**

**M.Sc., CHEMISTRY**  
**Choice Based Credit System**

Dr. Ambedkar Government Arts College (Autonomous) offers the Semester System of education with credits for PG courses. Credit is related to the number of hours a teacher teaches a particular subject as well as to the number of hours a student spends learning a subject or carrying out an activity. In the semester system of study, every academic year is divided into two semester sessions. Each semester will have a minimum of 90 working days and each day will have 5 working hours.

Differential weightage is given according to the content and duration of the courses in the curriculum design. Each course is designed variously under lectures/tutorials/laboratory work/seminar/project work/practical training/viva voce etc., to facilitate effective teaching and learning and the credits are assigned accordingly depending on the content and the specialization.

The minimum Credit requirement for a two year PG course shall be **91** (81 credits for Core and Elective and 10 credits for Soft skill papers & Internship).

**REGULATIONS**  
**(Effective from the academic year 2019-2020 and thereafter)**

**1. CONDITIONS FOR ADMISSION**

B.Sc., Chemistry with Mathematics / Physics and as one of ancillary subject.

**2. ELIGIBILITY FOR THE AWARD OF DEGREE**

A candidate shall be eligible for the award of the degree only if he/she has undergone the prescribed course of study in a college affiliated to the University for a period of not less than two academic years, passed the examination of all the four semester prescribed earning minimum of 91 credits and fulfilled such conditions as have been prescribed therefore.

**3. DURATION OF THE COURSE**

The duration of the course is for two academic years consisting of four Semesters.

#### 4. EXAMINATIONS

There shall be four semester examinations: first semester examinations at the middle of the first academic year and the second semester examination at the end of the first academic year. Similarly, the third and fourth semester examinations shall be held at the middle and the end of the second academic year , respectively.

#### 5. COURSE OF STUDY AND SCHEME OF EXAMINATIONS

The scheme of examinations for different semesters shall be as follows:

##### FIRST SEMESTER

| Course Components          | Subject Code | Subjects                    | Inst. Hours | Credits | Exam hours | Max. Marks |          | Total |
|----------------------------|--------------|-----------------------------|-------------|---------|------------|------------|----------|-------|
|                            |              |                             |             |         |            | CIA        | External |       |
| Core Paper-I               | 19PACHC1     | Inorganic Chemistry - I     | 6           | 4       | 3          | 25         | 75       | 100   |
| Core Paper-II              | 19PACHC2     | Organic Chemistry - I       | 6           | 4       | 3          | 25         | 75       | 100   |
| Core Paper-III             | 19PACHC3     | Physical Chemistry - I      | 6           | 4       | 3          | 25         | 75       | 100   |
| Core Paper-IV Practical-I* | -            | Organic Chemistry practical | 6           | -       | -          | 40         | 60       | 100   |
| Elective I                 | 19PACHE1     | Chemistry of Biomolecules   | 4           | 3       | 3          | 25         | 75       | 100   |
| Soft skills-I              | 19PASBE1     | Employability skills        | 2           | 2       | -          | 40         | 60       | 100   |
|                            |              | Total                       | 30          | 21      |            |            |          |       |

Practical Examinations shall be conducted at the end of even semester.

##### SECOND SEMESTER

| Course Components               | Subject Code | Subjects                                                   | Inst. Hours | Credits | Exam hours | Max. Marks |          | Total |
|---------------------------------|--------------|------------------------------------------------------------|-------------|---------|------------|------------|----------|-------|
|                                 |              |                                                            |             |         |            | CIA        | External |       |
| Core Paper-V                    | 19PBCHC1     | Inorganic Chemistry-II                                     | 5           | 4       | 3          | 25         | 75       | 100   |
| Core Paper-VI                   | 19PBCHC2     | Organic Chemistry - II                                     | 5           | 4       | 3          | 25         | 75       | 100   |
| Core Paper-VII                  | 19PBCHC3     | Physical Chemistry - II                                    | 5           | 4       | 3          | 25         | 75       | 100   |
| Core Paper-VIII Practical-I     | 19PBCHC4     | Physical Chemistry and Inorganic Chemistry practical       | 6           | 4       | 6          | 40         | 60       | 100   |
| Core Paper-IV Practical-I       | 19PBCHC5     | Organic Chemistry practical                                | 6           | 4       | 6          | 40         | 60       | 100   |
| Elective II                     | 19PBCHE1     | Modern synthetic strategies and renewable energy resources | 4           | 3       | 3          | 25         | 75       | 100   |
| Elective-Extra Disciplinary – I | 19PBCHD1     | Research Methodology                                       | 3           | 3       | 3          | 25         | 75       | 100   |
| Soft skills-II                  | 19PBSBE2     | Leadership & Computation Skills                            | 2           | 2       | -          | 40         | 60       | 100   |
|                                 |              | Total                                                      | 30          | 28      |            |            |          |       |

Practical Examinations shall be conducted at the end of even semester.

\* Internship will be carried out during the summer vacation of the second semester and the report will be evaluated by the two examiners within the Department of College/Institution. The marks should be sent to the Controller of Examinations and the same will be included in the Third semester marks statement.

### THIRD SEMESTER

| Course Components                | Subject Code | Subjects                      | Inst. Hours | Credits | Exam hours | Max. Marks |          | Total |
|----------------------------------|--------------|-------------------------------|-------------|---------|------------|------------|----------|-------|
|                                  |              |                               |             |         |            | CIA        | External |       |
| Core Paper-IX                    | 19PCCHC1     | Inorganic Chemistry-III       | 5           | 4       | 3          | 25         | 75       | 100   |
| Core Paper-X                     | 19PCCHC2     | Organic Chemistry - III       | 5           | 4       | 3          | 25         | 75       | 100   |
| Core Paper-XI                    | 19PCCHC3     | Physical Chemistry- III       | 5           | 4       | 3          | 25         | 75       | 100   |
| Core Paper-XII Practical-III     | -            | Inorganic Chemistry practical | 6           | -       | -          | 40         | 60       | 100   |
| Elective IV                      | 19PCCHE1     | Material Chemistry            | 4           | 3       | 3          | 25         | 75       | 100   |
| Elective-Extra Disciplinary - II | 19PCCHD2     | Biochemistry                  | 3           | 3       | 3          | 25         | 75       | 100   |
|                                  | 19PCINT1     | Internship*                   | -           | 2       | -          | -          | -        | 100   |
| Soft skills-III                  | 19PCSBE3     | Managerial Skills             | 2           | 2       | -          | 40         | 60       | 100   |
|                                  |              | Total                         | 30          | 22      |            |            |          |       |

Practical Examinations shall be conducted at the end of even semester.

### FOURTH SEMESTER

| Course Components            | Subject Code | Subjects                                         | Inst. Hours | Credits | Exam hours | Max. Marks |          | Total |
|------------------------------|--------------|--------------------------------------------------|-------------|---------|------------|------------|----------|-------|
|                              |              |                                                  |             |         |            | CIA        | External |       |
| Core Paper-XIII              | 19PDCHC1     | Organic Chemistry-IV                             | 6           | 4       | 3          | 25         | 75       | 100   |
| Core Paper-XIV               | 19PDCHC2     | Physical Chemistry-IV                            | 6           | 4       | 3          | 25         | 75       | 100   |
| Core Paper-XV Practical- IV  | 19PDCHC3     | Physical Chemistry & Organic Chemistry Practical | 6           | 4       | 6          | 25         | 75       | 100   |
| Core Paper-XII Practical-III | 19PDCHC4     | Inorganic Chemistry practical                    | 6           | 4       | 6          | 40         | 60       | 100   |
| Elective IV                  | 19PDCHE1     | Bioinorganic Chemistry                           | 5           | 3       | 3          | 25         | 75       | 100   |
| Elective-V                   | 19PDCHE2     | Environmental Chemistry                          | 5           | 3       | 3          | 25         | 75       | 100   |
| Soft skills-IV               | 19PDSBE4     | Personality Development                          | 2           | 2       | -          | 40         | 60       | 100   |
|                              |              | Total                                            | 30          | 24      |            |            |          |       |

Practical Examinations shall be conducted at the end of even semester.

The following procedure to be followed for Internal marks:

Theory: The break up for continuous Assessment is as follows.

- a) Test (2 x 20) : 40 Marks
- b) Assignment (2 x 10): 20 Marks
- c) Model Examination (1 x 40): 40 Marks

-----  
**100 Marks**  
 -----



100 Marks for continuous assessment can be converted to 25 Marks

Practical: Internal Marks: 40

|                              |          |
|------------------------------|----------|
| Model Examination            | 20 marks |
| Test (Best two out of three) | 30 marks |
| Record and Observation       | 50 marks |

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100 marks

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100 Marks for continuous assessment can be converted to 40 Marks

## **6. REQUIREMENT FOR PROCEEDING TO SUBSEQUENT SEMESTERS**

(i) Candidates shall register their names for the First semester examination after the admission in the PG courses.

(ii) Candidates shall be permitted to proceed from the First Semester upto the Final Semester irrespective of their failure in any of the Semester Examination subject to the condition that the candidates should register for all arrear subjects of earlier semester along with current (subject) Semester subjects.

(iii) Candidates shall be eligible to proceed to the subsequent semester, only if they earn, sufficient attendance as prescribed therefore by the Syndicate from time to time.

Provided in case of candidate earning less than 50% of attendance in any one of the semester due to any extraordinary circumstance such as medical grounds, such candidates who shall produce Medical Certificate issued by the Authorised Medical Attendant (AMA), duly certified by the Principal of the College, shall be permitted to proceed to the next semester and to complete the course of study. Such candidate shall have to repeat the missed semester by rejoining after completion of final semester of the course, after paying the fee for the break of study as prescribed by the University from time to time.

## **7. PASSING MINIMUM**

- There shall be no Passing Minimum for Internal.
- For External Examination, Passing Minimum shall be of 50% (Fifty Percentage) of the maximum marks prescribed for the paper.
- In the aggregate (External + Internal) the passing minimum shall be of 50% for each Paper/Practical and viva-voce.
- Grading shall be based on overall marks obtained (internal + external).

## 8. CLASSIFICATION OF SUCCESSFUL CANDIDATES

Candidates who secured not less than 60% of aggregate marks (Internal + External) in the whole examination shall be declared to have passed the examination in the First Class.

All other successful candidates shall be declared to have passed in Second Class.

Candidates who obtain 75% of the marks in the aggregate (Internal + External) shall be deemed to have passed the examination in First Class With Distinction, provided they pass all the examinations (theory papers, practicals, project and viva-voce) prescribed for the course in the First appearance.

## 9. GRADING SYSTEM

1. **Passing minimum** is 50% of the ESE and also 50% of the maximum of that paper/Course.
2. **Minimum Credits to be earned:** Best 90 Credits(Two year Programme)
3. Part A (80 Credits): Core, Elective,Non-major Electives and Extra Disciplinary and Part B ( 10 Credits) : Soft skills and Internship.
4. **Marks and Grades:**

The following table gives the marks, grade points, letter grades and classification to indicate the performance of the candidate.

**Conversion of Marks to Grade points and Letter Grade**  
**( Performance in a Paper/Course)**

| <b>RANGE OF MARKS</b> | <b>GRADE POINTS</b> | <b>LETTER GRADE</b> | <b>DESCRIPTION</b> |
|-----------------------|---------------------|---------------------|--------------------|
| 90-100                | 9.0 – 10.0          | O                   | Outstanding        |
| 80-89                 | 8.0 – 8.9           | D+                  | Excellent          |
| 75-79                 | 7.5 – 7.9           | D                   | Distinction        |
| 70-74                 | 7.0 – 7.4           | A+                  | Very Good          |
| 60-69                 | 6.0 – 6.9           | A                   | Good               |
| 50-59                 | 5.0 – 5.9           | B                   | Average            |
| 00-49                 | 0.0                 | U                   | Re-appear          |
| ABSENT                | 0.0                 | AAA                 | ABSENT             |

C<sub>i</sub> = Credits earned for course i in any semester.

G<sub>i</sub> = Grade point obtained for course i in any semester

‘n’ refers to the semester in which such courses were credited.

**For a Semester:**

$$\text{GRADE POINT AVERAGE[GPA]} = \frac{\sum_i C_i G_i}{\sum_i C_i}$$

$$\text{GPA} = \frac{\text{Sum of the multiplication of Grade points by the credits of the courses}}{\text{Sum of the credits of the courses in a semester}}$$

**For the entire programme:**

$$\text{CUMULATIVE GRADE POINT AVERAGE[CGPA]} = \frac{\sum_n \sum_i C_{ni} G_{ni}}{\sum_n \sum_i C_{ni}}$$

$$\text{CGPA} = \frac{\text{Sum of the multiplication of grade points by the credits of the entire programme}}{\text{Sum of the credits of the courses of the entire programme}}$$

| CGPA                        | GRADE           | CLASSIFICATION OF FINAL RESULT |
|-----------------------------|-----------------|--------------------------------|
| 9.5 – 10.0                  | O <sup>+</sup>  | First Class – Exemplary*       |
| 9.0 and above but below 9.5 | O               |                                |
| 8.5 and above but below 9.0 | D <sup>++</sup> |                                |
| 8.0 and above but below 8.5 | D <sup>+</sup>  | First Class with Distinction   |
| 7.5 and above but below 8.0 | D               |                                |
| 7.0 and above but below 7.5 | A <sup>++</sup> |                                |
| 6.5 and above but below 7.0 | A <sup>+</sup>  | First Class                    |
| 6.0 and above but below 6.5 | A               |                                |
| 5.5 and above but below 6.0 | B <sup>+</sup>  |                                |
| 5.0 and above but below 5.5 | B               | Second Class                   |
| 0.0 and above but below 5.0 | U               |                                |

\* The candidates who have passed in the first appearance and within the prescribed semester of the PG programme ( Core, Elective, Non major Electives and Extra Disciplinary course alone) are eligible.

## 10. RANKING

Candidates who pass all the examinations prescribed for the course in the **first appearance itself alone** are eligible for Ranking/Distinction.

Provided in the case of candidates who pass all the examinations prescribed for the course with a break in the First Appearance due to the reasons as furnished in the Regulations under “Requirements for Proceeding to subsequent Semester” are only eligible for Classification.

## 11. PATTERN OF QUESTION PAPER:

PART-A (50 words): Answer 10 Questions out of 12 Questions = 10 x 2 = 20 marks

PART-B (200 words): Answer 5 out of 8 Questions 5 x 5= 25 marks

**THE GENERAL OBJECTIVE**

*In the last few years, there is a great demand for Post Graduates in Chemistry in Pharma, Paint and Refinery industries. Chemistry has diversified into a multidisciplinary subject taking an active role in chemical and pharmaceutical industries, biotechnology and nano technology. Taking into consideration these facts, the syllabus of the M.Sc course is designed in such a way that a student would have a thorough knowledge on the fundamental aspects of chemistry and also expose himself/ herself to research. After completion of the course with a M. Sc. degree in Chemistry, he/she can have a career in the following areas: (i) take up a teaching job at the college for science and engineering courses, (ii) take up a job in a Scientific laboratory & R&D Institutions, (iii) pursue a research career in an academic institution or a National Institute/laboratory, (iv) even start one's own industry and be an entrepreneur. All the topics in the NET/SLET syllabus for Chemistry are incorporated, as passing the NET/SLET is a prerequisite for UGC/CSIR research fellowship and teaching jobs in Universities and several colleges and an added qualification for many research positions.*

## Semester – I

### CORE PAPER- I INORGANIC CHEMISTRY-I STRUCTURE AND BONDING

#### Objectives

- ❖ To provide knowledge of basic and advanced concepts in bonding and enable the students to identify the structure and bonding of simple molecules.
- ❖ To provide an understanding of the various types of solid state packing and the types of chemical forces
- ❖ To enable students appreciate the structure of inorganic chain and cluster compounds.
- ❖ To provide knowledge of the structure and bonding in boron compounds.

#### Expected outcomes

Students are able

- ✓ To identify the bonding types,
- ✓ To understand the structure and packing in solids
- ✓ To appreciate the structure of boranes, carboranes, metal clusters and inorganic polymers.

#### UNIT I: CHEMICAL BONDING

V.B. approach to bonding-Hitler-London, Pauling and Slater refinements, Concept of hybridization and structure of molecules, VSEPR theory shapes of molecules. M.O. approach to covalent bonding – symmetry and overlap of atomic orbitals – symmetry of molecular orbitals – sigma and pi bonding – energy levels in homo and hetero nuclear diatomic systems – bond length, bond order and bond energy, Application to small molecules such as  $\text{BeCl}_2$ ,  $\text{BCl}_3$  and  $\text{CCl}_4$ ,  $\text{SF}_4$ , etc, ionic character in a covalent bond - The concept of multicentre bonding. Pseudo halogens: Structure and bonding in  $\text{ClF}_3$ ,  $\text{BrF}_3$ ,  $\text{BrF}_5$ ,  $\text{IF}_5$ ,  $\text{IF}_7$  etc . Oxides and oxyacids of halogens, Bonding in Noble gas compounds –  $\text{XeCl}_2$ ,  $\text{XeF}_4$ ,  $\text{XeOF}_4$ ,  $\text{XeF}_6$ .

#### UNIT II: CHEMISTRY OF SOLID STATE I: STRUCTURE

Weak Chemical forces: van der Waals forces, Hydrogen bonding, Close packing of atoms and ions HCP and BCC types of packing voids, radius ratio – derivation – its influence on structures. Lattice energy – Born-Lande equation - Kapustinski equation, Madelung constant.

Representative structures of AB and  $\text{AB}_2$  types of compounds - rock salt, cesium chloride, wurtzite, zinc blende, rutile, fluorite, antiferite, cadmium iodide and nickel arsenide. Structure of graphite and diamond. Spinel -normal and inverse types and perovskite structures.

### UNIT III: CHEMISTRY OF SOLID STATE II: DIFFRACTION METHODS

Band theory of solids- non-stoichiometry- point defects – linear defects- effects due to dislocations-electrical properties of solids-conductor, insulator, semiconductor-intrinsic-impurity semiconductors-optical properties-lasers and phosphors-elementary study of liquid crystals.

Difference between point group and space group – screw axis – glide plane - symmetry elements – relationship between molecular symmetry and crystallographic symmetry – The Concept of reciprocal lattice – X-ray diffraction by single crystal – rotating crystal – powder diffraction. Neutron diffraction: Elementary treatment – comparison with X-ray diffraction. Electron diffraction- Basic principle. Crystal Growth methods: From melt and solution (hydrothermal, Gel methods).

### UNIT IV: BORON COMPOUNDS AND CLUSTERS

Chemistry of boron – boranes, higher boranes, borazines, boron nitrides, hydroborate ions – Preparation, properties and structure, STYX numbers, Wade's rules.

Carboranes- Types such as nido-closo, arachno-preaprtion properties and Structure. Metallocarboranes-a general study.Metal clusters: Chemistry of low molecularity metal clusters only, Structure of  $\text{Re}_2\text{Cl}_8$ ; multiple metal-metal bonds.

### UNIT V: INORGANIC CHAIN AND CLUSTER COMPOUNDS

Types of inorganic polymers, comparison with organic polymers, silanes, higher silanes, multiple bonded systems, silicon nitrides, siloxanes. P-N compounds, cyclophosphazenes and cyclophosphazanes. S-N compounds –  $\text{S}_4\text{N}_4$ ,  $(\text{SN})_x$ .

Isopoly and heteropoly acids – Structure and bonding of 6- and 12 – isopoly and heteropoly anions. Structure of silicates - applications of Paulings rule of electrovalence - isomorphous replacements in silicates – ortho, meta and pyro silicates – one dimensional, two dimensional and three dimensional silicates.

#### Reference and text books

1. D.E. Douglas, D.H. McDaniel and J.J. Alexander, Concepts and Models in Inorganic Chemistry, 3<sup>rd</sup> Ed, **1994**.
2. M.C. Day, J. Selbin, Theoretical Inorganic Chemistry, 2<sup>nd</sup> Ed, East West Press, **1985**.
3. L. Pauling, The Nature of the Chemical Bond, 3<sup>rd</sup> Ed., Cornell University Press, **1960**.
4. F.A. Cotton, G. Wilkinson, Advanced Inorganic Chemistry, 4<sup>th</sup> Ed, John Wiley & Sons, **1986**.
5. D.F. Shriver, P.W. Atkins, Inorganic Chemistry, 3<sup>rd</sup> Ed, **1999**.
6. A.G. Sharpe, Inorganic Chemistry, Pearson Education, **2008**.
7. N. H. Ray, Inorganic Polymers, Academic Press, **1978**.
8. A. R. West, Basic Solid State Chemistry, John Wiley, **1991**.
9. E.L. Mutteri, Polyhedral Boranes, Academic Press, NY, **1975**



## **CORE PAPER II ORGANIC CHEMISTRY –I**

### **REACTION MECHANISM AND STEREOCHEMISTRY**

#### **Objectives**

- ❖ Understanding the fundamental mechanism involved in electrophilic reactions, nucleophilic reactions and reactions that involve transient species.
- ❖ Understanding the basic aspects of stereochemistry such as chirality, nomenclature, stereoselectivity Vs stereospecificity and Asymmetric synthesis.
- ❖ Understanding the conformational analysis of six member ring systems.

#### **Expected outcomes**

- ✓ To enable the students to understand various types of reaction mechanisms involved in synthetic organic transformation.
- ✓ To enable the students to understand basic stereochemistry concept in a proper perspective.
- ✓ To enable the students to understand the concept of asymmetric synthesis.

#### **UNIT-I: REACTION MECHANISM**

Kinetic and Non kinetic methods of determining organic reaction mechanisms. Isolation and trapping of intermediates, Isotopic labeling studies. Primary Kinetic Isotopic effect. Generation of Kinetic and Thermodynamic enolates. Hammett equation-simple problems and Taft equation. Significance of reaction as well as substituent constants. Ambident nucleophiles such as  $\text{CN}^-$ ,  $\text{NO}_2^-$ , phenoxide and ambident dianions. Williamson's ether synthesis.

#### **UNIT-II: ALIPHATIC NUCLEOPHILIC SUBSTITUTION**

Mechanism of nucleophilic substitution reaction:  $\text{S}_\text{N}^1$ ,  $\text{S}_\text{N}^2$  and  $\text{S}_\text{N}^i$  mechanisms. Solvent and leaving group effects and neighbouring group participation (NGP). Substitution at carbonyl, vinylic and bridgehead system. Substitution with ambident nucleophiles- "O" Vs "C" alkylation. Role of LDA, crown ethers and phase transfer catalysts (PTC) in nucleophilic substitution reactions.

Generation of enolates, enolate selectivity (Kinetic Vs Thermodynamic), alkylation of enolates and stereochemistry of enolate alkylation. Mechanism of ester hydrolysis (only  $\text{BAC}^2$ ,  $\text{AAc}^2$  and  $\text{AAI}^1$ ). Alkylation of active methylene compounds. Asymmetric alkylation (Evans, Enders and Meyers procedures). Preparation and synthetic utility of enamines, Finkelstein reaction, Wurtz coupling.

### **UNIT-III: AROMATIC ELECTROPHILIC AND NUCLEOPHILIC SUBSTITUTIONS**

Aromatic electrophilic substitution: mechanism of nitration, sulfonation, Friedel-Crafts alkylation and acylation reactions. Synthesis of di- and tri-substituted benzenes from benzene or mono-substituted benzenes. Hammett and Hammett-Taft equation. Haworth reaction (for naphthalene), Scholl reaction, Vilsmeier-Haack formylation, Gattermann reaction, Reimer-Tiemann and Bischler-Napieralski reactions.

Aromatic nucleophilic substitution in aryl halides by Meisenheimer complex mechanism and benzyne mechanism. Reactions of aryl diazonium salts. Zeigler alkylation, Vicarious Nucleophilic Substitution (VNS), Chichibabin and Schiemann reactions.

### **UNIT-IV: REACTIVE INTERMEDIATES**

Organic reactive intermediates: Generation, stability and reactivity of carbocations, carbanions, free radicals, carbenes, carbenoids, benzyne and nitrenes.

### **UNIT-V: STEREOCHEMISTRY**

Chirality, Symmetry elements, Asymmetric and Dissymmetric chiral molecules. Calculation of number of optical isomers. Stereochemistry of mono and di-substituted cyclopropane, cyclobutane, cyclopentane and cyclohexane. Stereochemistry of tri-substituted cyclopentane, tri-substituted pentane and tetra-substituted hexane. Description of various types of optically active compounds including allenes, cumulenes, spiranes, biphenyls, *trans*-cyclooctene.

Compounds containing two asymmetric centers; Erythro and threo isomers. Conversion of Fischer projection into perspective forms. Erythro and Threo-Inter conversion of Fischer to Sawhorse and Newman projections. Zig-Zag representation of glucose. Interpretation of homotopic, enantiotopic and diastereotopic atoms and faces. Pro-chiral carbon. Concept of *Re*- and *Si*- faces. R & S nomenclature of simple compounds, allenes, spiranes and biphenyls. Stereospecific and Stereoselective reactions. Asymmetric Synthesis-Cram's rule and Felkin-Anh model. Conformational analyses of cyclohexane, di-substituted cyclohexanes and decalin.

### **Reference and text books**

1. Jerry March, Advanced Organic Chemistry, John Wiley & Sons, 5<sup>th</sup> Ed, **2001**.
2. F. Carey and R. J. Sundberg, Advanced Organic Chemistry-Part A and B, Springer Science + Business Media, 5<sup>th</sup> Ed, **2007**.

3. M. B. Smith and Jerry March, Advanced Organic Chemistry, John Wiley & Sons, 5<sup>th</sup> Ed, **2001**.
4. J. Clayden, N. Greeves and S. Warren, Organic Chemistry, Oxford University Press, 2<sup>nd</sup> Ed, **2012**.
5. R. O. C. Norman and J. M. Coxon, Principles of Organic Synthesis, Chapman & Hall, 3<sup>rd</sup> Ed, **1993**.
6. Stuart Warren, Organic Synthesis: Disconnection Approach, Wiley India (P) Ltd, **2007**.
7. I. L. Finar, Organic Chemistry Vol 2: Stereochemistry and the Chemistry of Natural product, Dorling Kindersley India (P) Ltd, **2009**.
8. E. N. Eliel, Stereochemistry of Carbon Compounds, Tata McGraw Hill Ed, Reprint **2008**.
9. D. Nasipuri, Stereochemistry of Organic Compounds, New Age International (P) Ltd, Reprint, **2005**.
10. Kalsi. P. S, Organic Reactions: Stereochemistry and Mechanism through solvedproblems, New AgeInternational (P)Ltd, 4<sup>th</sup> Ed, **2007**.
11. E. L. Eliel andS. H. Wilen, Stereochemistry of Organic Compounds, Wiley India Ed, **2008**.

## **CORE PAPER III PHYSICAL CHEMISTRY - I**

### **CHEMICAL KINETICS AND ELECTROCHEMISTRY**

#### **Objectives**

- ❖ To understand the kinetics of chemical kinetics and explore the reaction kinetics of fast reactions
- ❖ To learn the various techniques and mechanism of involved in catalysis.
- ❖ To gain on understanding of the Ionic activity, ionic interactions, Debye-Hückel-Bjerrum model, Debye-Hückel limiting law.
- ❖ To study the Debye-Hückel theory of strong electrolytes. To study the Electrical double layer, electrocapillary phenomena, surfactants.
- ❖ The design and applications of the batteries and Fuel Cells, Corrosion and its Protection.

#### **Expected outcomes**

- ✓ To understand and explore the reaction kinetics of fast reactions
- ✓ To learn the theory, kinetics and mechanism of enzyme catalysis.
- ✓ Understand concepts of Ionic interactions, theory of electrolytes, double layer models, Debye-Hückel limiting law.
- ✓ Understand the designs of Batteries, Fuel cells and ion selective electrodes

#### **UNIT-I: CHEMICAL KINETICS AND CATALYSIS**

Absolute reaction rate theory -Thermodynamic terms-Significance of entropy and volume of activation. Reactions in solution: factors determining reaction rates in solutions, effect of dielectric constant and ionic strength, - Bronsted -Bjerrum equation-Primary and Secondary salt effect, influence of solvent on reaction rates. Acid base catalysis-Bronsted relations, catalytic coefficients and their determination.

#### **UNIT-II: CHEMICAL DYNAMICS**

Potential energy surfaces-Dynamics of unimolecular reactions-Lindemann Hinshelwood, Rice-Ramsperger-Kassel(RRK) theory.Rice-Ramsperger-Kassel -Marcus (RRKM) theory.

Study of fast reactions by stopped flow techniques- relaxation method, flash photolysis and the nuclear magnetic resonance method.

Linear free energy relationship-Hammett equation, Taft equation-Separation of polar, resonance and steric effects.

### **UNIT-III: ENZYME CATALYSIS**

Enzyme catalysis and its mechanism, Michaelis-Menten equation, effect of pH and temperature on enzyme catalysis, Mechanism of enzyme inhibition kinetics of surface reactions- unimolecular reactions-Bimolecular reactions-Langmuir Hinshelwood and Eley-Rideal mechanism.

### **UNIT IV: ELECTROCHEMISTRY - I**

Deviation from ideal behaviour.ion-solvent and ion-ion interactions. Debye-Hückel-Bjerrum model, Ion association and triple ion formations.Expression for the mean activity coefficient.Debye-Hückel limiting law and its applications -Diverse ion effect.Van't Hoff factor and its relation to colligative properties.Debye-Hückel theory of strong electrolytes.Debye-Hückel length and potential around a central ion, its interpretation. Transport of ions in Solution: Electrolytic conduction- Debye - Hückel-Onsager treatment of strong electrolytes- ionic atmosphere- Anomalous conductance of non aqueous electrolytes.

### **UNIT V: ELECTROCHEMISTRY- II**

Electrical double layer - Electrocapillary phenomena - Surfactants - Lipmann's equation, Electrokinetic phenomena.Zeta potential and its applications.Structure of electrical double layer – Helmholtz-Perrin, Guoy-Chapmann and Stern models. Butler-Volmer equation for one electron transfer reaction - equilibrium and exchange current densities- and symmetry factor - transfer coefficient.Cyclic voltammetry and Stripping voltammetry - principle – instrumentation- Corrosion and passivation of metals - Pourbaix diagram - Evans diagram –Batteries and Fuel cells-Ion selective electrodes.

### **Reference and text books**

1. K.J.Laidler, Chemical Kinetics, Harper and Row, New York,**1987**.
2. R.G. Frost and Pearson, Kinetics and Mechanism, Wiley New York, **1961**.
3. A.W.Anderson, Physical Chemistry of Surfaces, Wiley - Interscience, Newyork, 1990.
4. Paula, Peter Atkins and Julio de, Elements of Physical chemistry, 5th Ed, Oxford U.P,**2012**.
5. Mordechay Schlesinger, Modern Aspects of Electrochemistry: Issue 43, Springer, Netherlands, **2009**.
6. J. N. Gurtu and A. Gurthu, Advanced Physical Chemistry, Pragathi Prakashan, Meerut, Revised, **2014**.

## **CORE PAPER-IV**

### **Organic Chemistry Practical**

#### **OBJECTIVES:**

This comprises of TWO parts

#### **I. Analysis of a mixture of organic Compounds.**

The practical is designed as to give the students exposure to lab techniques in analysis of organic molecules and organic compounds.

1. Identification of components in a two component mixture and preparation of their derivatives.
2. Determination of b.p./ m.p. for components and m.p. for the derivatives.

#### **II. Single stage organic preparations illustrating various types of reactions.**

1. Salicylic acid from methyl salicylate(Hydrolysis)
2. 2,4,6-Tribromoaniline from aniline (Bromination)
3. m-Dinitrobenzene from nitrobenzene (Nitration)
4. Acetanilide from aniline (Acetylation)
5. 2-Naphthyl benzoate from 2-naphthol (Benzoylation)
6. Benzoic acid from Benzyl alcohol (Oxidation)
7. Diethyl oxalate from oxalic acid ( Esterification)
8. Sulphanilic acid from aniline (Sulphonation)

## **ELECTIVE-I**

### **METALLO PROTEINS, METALLO ENZYMES, AMINO ACIDS, PROTEINS, NUCLEIC ACIDS, CARBOHYDRATES, ANTIBIOTICS, VITAMINS AND SEPARATION TECHNIQUES**

#### **Objectives**

- ❖ To have a knowledge about protein metallo biomolecules and the role of metal ions in biological process.
- ❖ To learn about chemical toxicology and uses of inorganic compounds as therapeutic agents.
- ❖ To learn about storage and transport of metal ions in biological system
- ❖ To learn about polymeric bio-organic molecules such as carbohydrates, proteins and nucleic acids.
- ❖ To learn about the structure, stereochemistry and synthesis of antibiotics and vitamins.
- ❖ To learn about various types of separation techniques for organic and biomolecules.

#### **Expected outcomes**

- ✓ To enable the students to understand the importance of Fe, Mg and Cu-containing proteins.
- ✓ To enable the students to understand the structure and functions of various types of metallo enzymes.
- ✓ To enable the students to understand the importance of trace elements in biological system and also the toxicity of metal ions.
- ✓ To enable the students to understand the role of metals in medicine.
- ✓ To enable the students to understand the importance of transport and storage metals in biological systems.
- ✓ To enable the students to understand the structure and importance of biomolecules such as proteins, nucleic acids and carbohydrate.
- ✓ To enable the students to understand the structure and importance of antibiotics and vitamins.
- ✓ To enable the students to learn the various types of separation techniques involved in organic as well as bio-organic molecules.

#### **UNIT-I: METALLO PROTEINS**

**Iron containing proteins:** Metalloporphyrins-Haemoglobin and myoglobin – Structures and work functions – synthetic oxygen carriers – Cytochrome – structure and work function. Non heme oxygen carriers – Electron carrier proteins – Iron sulphur proteins.

**Magnesium containing proteins:** Chlorophyll – structure – photosynthetic sequence.

**Copper containing proteins:** Classification – blue copper proteins – structure of blue copper electron transferases – copper protein as oxidases – cytochrome c oxidase – mechanistic studies of cytochrome c oxidase

## **UNIT II: METALLO ENZYMES**

**Metallo enzymes:** Carboxy peptidase A – structure and function ; Carbonic anhydrase – inhibition and poisoning – Corrin ring system – Vitamin B<sub>12</sub> ( cyanocobalamin ) and B<sub>12</sub> coenzymes – In vivo and In vitro nitrogen fixation. **Essentials of trace elements and chemical toxicology:** Trace elements in biological system. Metal ion toxicity - classes of toxic metal compounds – detoxification. **Metals in medicine:** Anti arthritis drugs – Au and Cu in rheumatoid arthritis – Li in psychiatry – Pt, Au and metallocenes in anti cancer drugs- metals in radiodiagnosis and magnetic resonance imaging. **Transport and storage of metals:** Mechanism – Fe, Cu, Zn and V storage and transport – metallothioneins. Molecular mechanism of iron transport across the membrane – sodium and potassium ion pumps.

## **UNIT-III: AMINO ACIDS AND PROTEINS, NUCLEIC ACIDS AND CARBOHYDRATES**

**Amino acids and Proteins:** Amino acids and Protein structure, Analysis of N-terminal and C-terminals in a polypeptide. Sanger method, Edman degradation and Enzymatic analysis. Primary, secondary and tertiary structure of proteins. **Nucleic acids and Carbohydrates:** Chemistry of nucleic acids, nucleosides and nucleotides – Structure RNA and DNA and their biological importance. Pyranose and furanose forms of aldohexose and ketohexose – methods used for the determination of ring size - conformation of aldohexopyranose – structure and synthesis of lactose and sucrose. A brief study of starch and cellulose.

## **UNIT-IV: ANTIBIOTICS AND VITAMINS**

**Biomolecules: Antibiotics and vitamins:** A detailed study of structure, stereochemistry and synthesis of penicillin, cephalosporin. Chemistry and physiological action of ascorbic acid, thiamin, riboflavin and pyridoxine – Elementary aspect of vitamin A, E, K and B<sub>12</sub>.

## **UNIT V: SEPARATION TECHNIQUES**

Basic aspects of thin-layer chromatography (TLC), column chromatography and flash vacuum column chromatography. Principles, theory, instrumentation and applications of Ion-exchange column Chromatography, Gel-permeation Chromatography, Gas chromatography



and High Performance Liquid chromatography (HPLC)-Interpretation of chromatogram and separation of components from the mixture.

### **Reference and text books**

1. S. J. Lippard and J. M. Berg, Principles of Bioinorganic Chemistry, Panima Publishing Corporation, **1997**.
2. W. Kaim and B. Schwederski, Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, (An Introduction and Guide), John Wiley and Sons, **1994**.
3. J. E. Huheey, E. A. Keiter and R. L. Keiter, Inorganic Chemistry, Principles of Structure and Reactivity, Pearson Education, **2004**.
4. F. A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, Wiley Eastern, 5<sup>th</sup> Ed, **1998**.
5. David L. Nelson and Michael M. Cox, Leninger Principles of Biochemistry, WH Freeman, **2017**.
6. I. L. Finar, Organic Chemistry Vol 2, Stereochemistry and the Chemistry of Natural Product, Dorling Kindersley India (P) Ltd, **2009**.
7. Douglas A. Skoog, F. James Holler and Stanley R. Crouch, Principles of Instrumental Analysis, CENAGE Learning, 7<sup>th</sup> Ed, **2018**.
8. D. A. Skoog and D. M. West, Fundamentals of Analytical Chemistry, Holt Rinehart and Winston Publications, 4<sup>th</sup> Ed, **1982**.

## **SEMESTER – II**

### **CORE PAPER V INORGANIC CHEMISTRY - II COORDINATION CHEMISTRY**

#### **Objectives**

- ❖ To learn about thermodynamic and stereochemical aspects of complex formation
- ❖ To learn about Various theories of complexes and their magnetic properties
- ❖ To learn about term symbols and energy level diagram of weak and strong field ligands, charge transfer spectra and spectral properties of lanthanides and actinides.
- ❖ To learn about various mechanisms of substitution and electron transfer reactions.
- ❖ To study the recent development in the catalysis

#### **Expected outcomes**

Students gain knowledge about

- ✓ Stability constant, types of macrocyclic ligands and nomenclature of chiral complexes
- ✓ Evaluating the value of  $Dq$  and  $B$  values with the help of Orgel diagrams
- ✓ Distortion in co-ordination complexes concept of sigma and pi bonding in complexes,
- ✓ Application of substitution reactions in the synthesis of Platinum and Cobalt complexes
- ✓ The use of catalytic activity of co-ordination complexes in the synthesis of organic compounds.

#### **UNIT-I: STABILITY OF COMPLEXES**

Stability of complexes- Factors affecting stability of complexes, Thermodynamic aspects of complex formation, Stepwise and overall formation constants, Stability correlations, statistical factors and chelate effect, Determination of stability constant and composition of the complexes: Formation curves and Bjerrum's half method, Potentiometric method, Spectrophotometric method, Ion exchange method, Polarographic method and Continuous variation method (Job's method)

Stereochemical aspects- Stereoisomerism in inorganic complexes- Isomerism arising out of ligand distribution and ligand conformation, Chirality and nomenclature of chiral complexes; Application of ORD and CD in the identification of complexes.

Macrocyclic ligands- Porphyrins, Corrins, Schiff's bases, crown ethers, etc.

#### **UNIT-II: METAL LIGAND BONDING**

Crystal field theory – Splitting of d orbitals under various geometries - factors affecting splitting, CFSE, evidences for CFSE (Structural and thermodynamic effects), spectrochemical series, Jorgensen relation, site preferences, Jahn Teller distortion – Dynamic and Static J.T. effect, Jahn Teller effect and chelation, Application of CFT – Magnetic properties, spectral properties and Kinetic properties, Limitations of CFT, Evidences for M-L overlap.

MOT – MO theory and energy level diagrams concept of Weak and strong fields, Sigma and pi bonding in octahedral, square planar and tetrahedral complexes. Nephelauxetic effect, Magnetic properties of complexes. Comparison of CFT and MOT of bonding in octahedral complexes.

### **UNIT-III: ELECTRONIC SPECTRA OF COMPLEXES**

Spectroscopic term symbols for  $d^n$  ions – derivation of term symbols and ground state term symbol, Hund's rule, Selection rules – breakdown of selection rules, spin orbit coupling, band intensities, weak and strong field limits – correlation diagram, Energy level diagrams. Orgel diagram for weak field Oh and Td complexes – Splitting of energy level due to Jahn-Teller distortion. Modified Orgel diagram – Limitations of Orgel diagram Tanabe–Sugano (T-S) diagrams – Evaluation of  $Dq$  and  $B$  values for  $d^2$ – $d^8$  complexes charge transfer spectra. Complications in band classification between Lf(d-d) and CT bands. Comparison between d-d bands and CT bands – Numerical problems, Lanthanides and Actinides- Spectral properties.

### **UNIT IV: INORGANIC REACTION MECHANISM**

Electron transfer reactions – Inner sphere (ISET) and outer sphere (OSET) electron transfer processes.. Role of bridging ligand with ISET reaction – tunneling transfer – multiple bridging in the activated complex in the ISET process. Complimentary and non complimentary ET reactions. Cross reactions and Marcus Hush theory.

Reaction mechanism of coordination compounds – Types of ligand substitution reactions – mechanism; Dissociative mechanism (D), Associative mechanism (A) interchange mechanism (I), Labile and Inert complexes. Substitution Reaction in octahedral complexes – general mechanism, general rate law for A, D and I - distinction between D, Id, IA pathways, replacement of coordinated water, mechanism of acid hydrolysis, base hydrolysis – DCB mechanism – direct and indirect evidences in favour of the mechanism. Ligand substitution reactions without cleavage of M-L Bond. Anation Reactions. Substitution in square planar complexes – General mechanism, Trans effect, influences of entering and leaving groups. Application of trans effect – synthesis of isomers of  $pt(II)$  complexes – theories of trans effect and cis-trans isomerisation reaction. Application of substitution reactions in the synthesis of Platinum and Cobalt complexes.

## UNIT-V: CATALYSIS

General principles of catalysis – basic reactions involved in the catalysis by organometallic compounds. Hydrogenation of olefins (Wilkinson's catalyst) ; Hydroformylation of olefins using Cobalt or Rhodium catalysts (OXO process); oxidation of olefins to aldehydes and ketones (wacker process) Monsanto acetic acid synthesis from methanol. Cyclooligomerisation of acetylene using Ni catalyst (Reppé's catalyst) Synthetic gasoline by using ZSM-5 catalyst (Fisher-Tropsch and mobil process) polymerization of olefins (Zeigler – Natta Catalyst), polymer bound catalyst.

### Reference and text books

1. H. J. Emelius and Sharpe, Modern aspects of Inorganic chemistry, Universal book stall, New Delhi, **1989**.
2. J. E. Huheey, E.A. Keiter and R.L. Keiter, Inorganic chemistry-Principles on structure and reactivity, 4<sup>th</sup> Ed, Pearson- education, **2002**.
4. F. A. Cotton and G. Wilkinson Advanced Inorganic Chemistry, Wiley Eastern, **1988**.
5. K. F. Purcell and J. C. Kotz, Inorganic Chemistry, WB Sanders Co, USA, **1977**.
7. D. F. Shriver, P. W. Atkins and C. H. Longford, Inorganic Chemistry, ELBS, 2<sup>nd</sup> Ed, **1994**.
8. D. Bannerjee, Co-ordination Chemistry, TATA Mcgraw Hill, **1993**.
10. M. L. Tobe, Inorganic Reaction Mechanism, Nelson, **1972**.
11. K. Burjer, Co-ordination Chemistry Experimental Methods, Butterworths, **1973**.

## CORE PAPER VI ORGANIC CHEMISTRY - II REACTION MECHANISM, REARRANGEMENT, NAME REACTIONS, OXIDATION AND REDUCTION

### Objectives

- ❖ Understanding addition and elimination reactions along with their mechanism and synthetic utility.
- ❖ Understanding rearrangement and name reactions along with their mechanism and synthetic utility.
- ❖ Understanding various types of oxidation and reduction reactions along with their mechanism and synthetic utility.

### Expected outcomes

- ✓ To enable the students to understand reaction mechanisms involved in additions, and elimination reactions.
- ✓ To enable the students to understand reaction mechanisms involved in rearrangements as well as name reactions along with their synthetic utilities.
- ✓ To enable the students to understand various types of oxidation and reduction reactions along with their synthetic utilities.

## **UNIT-I: ADDITION TO CARBON-CARBON DOUBLE BOND**

Electrophilic addition to carbon-carbon double and triple bonds. Nucleophilic addition to carbon-carbon multiple bonds. Generation and addition of carbenes-Michael addition and Robinson annulation.

Hydroxylation of olefinic double bonds ( $\text{OsO}_4$ ,  $\text{KMnO}_4$ ); Woodward and Prevost oxidation. Epoxidation using peracids including Sharpless epoxidation, Ozonolysis. Hydrogenation (homogenous and heterogeneous) and Transfer hydrogenation. Hydration of carbon-carbon double and triple bonds.

## **UNIT-II: ADDITION TO CARBON-OXYGEN DOUBLE BOND**

Nucleophilic addition to  $\text{C}=\text{O}$  bond. A study of Mannich, benzoin, Darzen's glycidic ester, Stobbe and Knoevenagel condensation reactions; Wittig, Wittig-Horner olefination reactions; Sulfur and Sulfonium ylides and their reactions, Julia olefination & Peterson alkene synthesis. Asymmetric reduction of carbonyl functions (Corey's procedure).

## **UNIT-III: ELIMINATION**

Elimination reactions:  $\text{E}_1$ ,  $\text{E}_2$ ,  $\text{E}_{1\text{cb}}$  and  $\text{E}_{\text{i}}$ -elimination. Conformation of mechanism; solvent, substrate, leaving group effects-Saytzeff's Vs Hoffman elimination; Stereochemistry of  $\text{E}_2$  eliminations, Elimination in cyclohexane ring system; Mechanism of pyrolytic eliminations. Examples: Chugaev reactions and Cope elimination, Hoffmann degradation and pyrolysis of esters.

## **UNIT-IV: MOLECULAR REARRANGMENTS & NAME REACTIONS**

A study of mechanism of the following rearrangements: Beckmann, Curtius, Hofmann, Schmidt, Lossen, Wolff, Pinacol, Wagner Meerwin, Demjanov, Dienone-Phenol, Favorski, Benzidine, Claisen, Cope, Sommelet-Hauser, Pummerer and Von-Richter rearrangements.

A study of the following name reactions: Dieckmann cyclization, Hofmann-Löffler Freytag reaction, Mitsunobu reaction, Shapiro reaction, Eschenmoser-Tanabe and Ramburg-Backlund reactions.

## **UNIT-V: OXIDATION AND REDUCTIONS REACTIONS**

Oxidation with Cr (including PCC, PDC, Jones) and Mn (including  $\text{MnO}_2$  and  $\text{BaMnO}_4$ ) reagents; Oxidation with LTA, DDQ and  $\text{SeO}_2$ ; Oxidation using DMSO either with DCC or  $\text{Ac}_2\text{O}$  or Oxaloyl chloride; Oxidation using IBX and Dess-Martin Periodinane (DMP) reagent.

Reduction with  $\text{NaBH}_4$ ,  $\text{NaCNBH}_3$ ,  $\text{Zn}(\text{BH}_4)_2$ ,  $\text{LiAlH}_4$ ,  $\text{Li}(\text{tBuO})_3\text{AlH}$ , DIBAL-H, Red-Al,  $\text{Et}_3\text{SiH}$  and  $\text{Bu}_3\text{SnH}$ ; Reduction using selectrides; Birch reduction.

### Reference and text books

1. Jerry March, Advanced Organic Chemistry, John Wiley & Sons, 5<sup>th</sup> Ed, **2001**.
2. F. Carey and R. J. Sundberg, Advanced Organic Chemistry-Part A and B, Springer Science + Business Media, 5<sup>th</sup> Ed, **2007**.
3. M. B. Smith and Jerry March, Advanced Organic Chemistry, John Wiley & Sons, 5<sup>th</sup> Ed, **2001**.
4. J. Clayden, N. Greeves and S. Warren, Organic Chemistry, Oxford University Press, 2<sup>nd</sup> Ed, **2012**.
5. M. B. Smith, Organic Synthesis, Academic Press, 3<sup>rd</sup> Ed, **2011**.
6. R. O. C. Norman and J. M. Coxon, Principles of Organic Synthesis, Chapman & Hall, 3<sup>rd</sup> Ed, **1993**.
7. Stuart Warren, Organic Synthesis: Disconnection Approach, Wiley India (P) Ltd, **2007**.
8. V. K. Ahluwalia, Oxidation in Organic Synthesis, CRC Press, 1<sup>st</sup> Ed, **2012**.
9. V. K. Ahluwalia, Reduction in Organic Synthesis, CRC Press, 1<sup>st</sup> Ed, **2012**.

## **CORE PAPER VII PHYSICAL CHEMISTRY - II**

### **QUANTUM CHEMISTRY AND ANALYTICAL TECHNIQUES**

#### **Objectives**

- ❖ To learn the principles of quantum mechanics of simple systems.
- ❖ To learn the quantum mechanical treatment of multi electron atoms.
- ❖ To learn the principles, instrumentation, interpretation and applications of micro wave, IR and Raman spectroscopy.
- ❖ To learn the principles, instrumentation and applications of Polarography, Amperometry, Coulometry
- ❖ To understand the principles, instrumentation and applications of various thermal analysis techniques
- ❖ To understand the principles, instrumentation and applications of various elemental analysis and surface analysis techniques

#### **Expected outcomes**

After completing this course, the students will

- ✓ learn the principles and postulates of quantum mechanics of simple systems.
- ✓ learn the quantum mechanical treatment of multi electron systems.
- ✓ Be able to calculate the energy of simple multi-electron atoms and molecules
- ✓ Understand the principles, instrumentation, interpretation and applications of micro wave, IR and Raman spectroscopy
- ✓ Understand the principles, instrumentation and applications of Polarography, Amperometry, Coulometry
- ✓ Understand the principles, instrumentation and applications of various thermal analysis techniques
- ✓ Understand the principles, instrumentation and applications of various elemental analysis and surface analysis techniques

#### **UNIT-I: QUANTUM CHEMISTRY-I**

Black body radiation-Planck's quantum theory-Wave particle duality-Uncertainty Principle. Operators-linear, commutation, Hermitian and Hamiltonian operators. Eigen functions and Eigen values-Postulates of quantum mechanics. Derivation of Schrodinger's time-independent wave equation and its application to particle in a one dimensional box, particle in a three dimensional box, harmonic oscillator, rigid rotor and hydrogen atom.

## **UNIT-II: QUANTUM CHEMISTRY-II**

Born-Oppenheimer approximation-Hydrogen molecule ion.LCAO-MO and VB treatments of the hydrogen molecule.Antisymmetry and Pauli's exclusion principle. Slater detrimental wave function, term symbols and spectroscopic states-Russell Saunders coupling.

The variation theorem and Perturbation theory.Applications of variation method and perturbation theory to the helium atom.Hybridization-determination of bond angles of sp, sp<sup>2</sup> and sp<sup>3</sup> hybridizations.Huckel pi electron (HMO) theory and its applications to ethylene, butadiene and benzene. A brief idea of Hartree and Hartree-Fockself consistent field theory.

## **UNIT III: ROTATIONAL SPECTROSCOPY**

Micro wave spectroscopy- Theory- selection rules, –Instrumentation; Energy levels in atoms and molecules- Fourier transformation Rotational spectra of diatomic and polyatomic molecules–P,Q,R branches- effect of isotopic substitution. Non-rigid rotator-Linear molecules.Theory of Rotational Raman spectra.

## **UNIT IV: VIBRATIONAL SPECTROSCOPY**

Vibrational spectra of diatomic molecules – – selection rules –overtones, combination and hot bands - Fermi resonance Energy of diatomic molecule, simple harmonic and unharmonic oscillator, rotational character of vibration spectra, Theory of Vibrational Raman spectroscopy-CoherentAntistokes Raman Spectroscopy (CARS).

## **UNIT V: ANALYTICAL TECHNIQUES**

Principles, theory, instrumentation and applications of Polarography, amperometry, coulometry, EDAX, XPS, AAS, AES, interpretation of spectra-Merits and demerits.

### **Reference and text books**

1. P.W. Atkins, Molecular Quantum Mechanics, Oxford University Press, Oxford, **1983**.
2. M.W.Hanna, Quantum Mechanics in Chemistry, W.ABenjamin Inc. London **1965**.
3. H. Eyring, J. Walter and G.Kimball, Quantum Chemistry, John Wiley and Sons, New York, **1944**.
4. G.M.Barrow, Introduction to Molecular Spectroscopy, McGrawHill, NewYork, **1988**.
5. D. A. McQuarrie, Quantum Chemistry, University Science Books, MilValley, California, **1998**.
6. A.K. Chandra, Introduction to Quantum Chemistry, Tata McGraw Hill, **1997**.
7. W. Levine, Quantum Chemistry, Prentice Hall, **1994**.
8. R. K. Prasad, Quantum Chemistry, Wiley Eastern, **1993**.
9. C.F. Banwell, Fundamentals of Molecular Spectroscopy, McGraw Hill, New York, **1966**.
10. R.S. Drago, Physical methods in chemistry, Reinhold, New York,**1968**.



**Core Paper VIII Practical – II Subject Code:**  
**Physical Chemistry & Inorganic Chemistry Practical**

**PHYSICAL CHEMISTRY PRACTICAL:**

**KINETICS:**

1. Kinetic study and comparison of acid strengths using acid catalysed hydrolysis of methyl acetate.
2. Determination of the rate constant and order for the reaction between potassium persulphate and potassium iodide.

**PHASE STUDY:**

3. Construction of phase diagram for a simple binary system : naphthalene – biphenyl, naphthalene –p-dichlorobenzene , naphthalene-diphenylamine.

**DISTRIBUTION LAW:**

4. Determination of equilibrium constant of the reaction between iodine and potassium iodide by partition method.
5. Determination of the concentration of given potassium iodide solutions by partition method.
6. Determination of molecular weight of benzoic acid in benzene and the degree of association of benzoic acid in benzene using partition method .

**ADSORPTION STUDY:**

7. Study of the adsorption of acetic acid or oxalic acid on charcoal , verification of Freundlich isotherm and determination of concentration of given acetic acid or oxalic acid.

**CONDUCTOMETRY:**

8. Determination of strength of strong acid and weak acid present in a mixture.
9. Determination of equivalent conductance of a strong acid at different concentrations .

**POTENTIOMETRY:**

10. Determination of pH and  $pK_a$  values using quinhydrone electrode.
11. Determination of the strength of KI solution using  $KMnO_4$  as link solution.

**INORGANIC CHEMISTRY PRACTICAL:**

1. Qualitative analysis employing semimicro methods and spot tests of mixtures of common cations plus ions containing the following less familiar elements W, Se, Te, Mo, Ce, Th, Ti, Zr, U, Be, V and Li.
2. Preparation of the following complexes:-  
Potassium trioxalatoferrate (III) trihydrate.  
Hexamminecobalt (III) Chloride, Potassium trisoxalatochromate (III)  
Thiourea complexes of copper(I)  
Tetramminecopper (II) Sulphate
3. Complexometric Titrations using EDTA.  
Estimation of  $Mg^{2+}$ ,  $Zn^{2+}$  and  $Ca^{2+}$

## **ELECTIVE-II**

### **MODERN SYNTHETIC STRATEGIES, GREENCHEMISTRY ANDRENEWABLE ENERGY RESOURCES**

#### **Objectives**

- ❖ To understand the basic aspects of organic reactions in terms of acceptor and donor synthons.
- ❖ To understand retrosynthetic analysis and various types of organic syntheses involved in accessing natural products.
- ❖ To understand the mechanism and synthetic utility of transition metal catalyzed organic reactions.
- ❖ To understand the concept of asymmetric synthesis and their applications.
- ❖ To understand various types of total synthesis involved in natural products.
- ❖ To understand the advantages of green reactions and their utility.

#### **Expected outcomes**

- ✓ To enable the students to understand reaction reactions in terms of donors and acceptor synthons.
- ✓ To enable the students to understand retro-synthetic analysis for simple organic compounds.
- ✓ To enable the students to understand the mechanism and synthetic utility of transition metal catalyzed reactions.
- ✓ To enable the students to followthe concept of asymmetric synthesis and their applications.
- ✓ To enable the students to learn different types of total syntheses involved in accessing natural products.
- ✓ To enable the students to learn the principles of green chemistry, green synthesis and isolation of bioactive compounds, green catalysis and renewable energy systems.

#### **UNIT-I: SYNTHETIC METHODOLGY**

Synthons (acceptor and donor)-Retrosynthetic analysis-Discoconnection approach Umpolung, antithesis, 1,3-Dipolar cycloaddition methodologies (Azide, nitrile oxide, azomethine ylides and carbonyl ylides). Concept of Tandem, cascade and domino reactions in organic synthesis. Various types of cyclization and ring formation reaction: anionic, cationic, radical and transition metal mediated cyclizations.

#### **UNIT-II: NOVEL REAGENTS AND ASYMMETRIC SYNTHESIS**

Role of palladium and nickel catalysts in organic reactions including Pd(0), Ni(0), Pd(II) and Ni(II) complexes. Typical reactions involving Heck, Negishi, Suzuki-Miyaura,

Kumada, Sonogashira, Stille and Hiyama coupling for carbon-carbon bond formation reactions. Buchwald-Hartwig coupling for the carbon-heteroatom bond formation reactions.

Selectivity, Resolution-Kinetic resolution reactions, Desymmetrization, Asymmetric induction, Chiral auxiliary. Generation of Asymmetric synthesis-Substrate-Auxiliary-Reagent and Catalyst control. Auxiliary controlled alkylation of chiral enolates, Evans oxazolidones, chiral hydrozones and chiral imines. Enders RAMP/SAMP and chiral sulfoxide. Asymmetric oxidation [dihydroxylation, epoxidation Sharpless, Jacobsen, Shi] and Asymmetric reduction (Noyori, Corey, Pfaltz)-Boranes reduction.

### **UNIT-III: TOTAL SYNTHESIS OF NATURAL PRODUCTS**

Classification of Organic Synthesis. Demonstration of various types of total syntheses using alkaloid (Epibatidine and Ibogamine), Prostaglandin (PGE<sub>1</sub>) and Terpenes (longifolene and cedrene)

### **UNIT-IV: ESSENTIALS OF GREEN CHEMISTRY**

Introduction to green chemistry-definition, origin, history, needs, goals, twelve principles of green chemistry. Usage of Conventional and Green solvents-Advantages, Limitations and drawbacks. Green Synthesis – Designing, Choice of starting materials, choice of reagents, choice of catalysts: bio catalysts, polymer supported catalysts, choice of solvents. Synthesis involving basic principles of green chemistry. Examples: synthesis of adipic acid, methyl methacrylate, paracetamol. Microwave, Ultrasonication and Ultrasound assisted reactions – esterification, reduction AND coupling reactions.

### **UNIT-V: RENEWABLE ENERGY RESOURCES**

Renewable energy sources: types of renewable energy sources. Solar cells: basic principles, types and their applications. Fuel cells: basic principles, types and their applications. Working principle and applications of Biofuel cells-brief introduction about hydroelectric, biomass, wind power and geothermal power and their applications and limitations-energy from some other natural source.

#### **Reference and text books**

1. R. O. C. Norman and J. M. Coxon, Principles of Organic Synthesis, Chapman & Hall, 3<sup>rd</sup> Ed, **1993**.
2. R. E. Gawley & J Aube, Principles of Asymmetric Synthesis, Elsevier, 2<sup>nd</sup> Ed, **2012**.
3. I. L. Finar, Organic Chemistry Vol 2, Stereochemistry and the Chemistry of Natural Product, Dorling Kindersley India (P) Ltd, **2009**.
4. V. K. Ahluwalia, Methods and Reagents of Green Chemistry: An Introduction by Green Chemistry, Kluwer Academic Publisher & Anamaya Publishers, **2004**.

**EXTRA DISCIPLINARY ELECTIVE COURSE – I**  
**RESEARCH METHODOLOGY**

**Unit I**

Meaning of research-purpose and objective of research-steps in research (scientific approach)- types of research –analytical, applied, qualitative and qualitative, empirical research-significance of research-research methods and methodology- criteria of good research-qualification of a researcher-problems encountered by researchers in india.

**Unit -II**

Sources of literature - primary, secondary and tertiary sources. Research problems - selecting the problem - necessity of defining the problem.

Data collection-collection of primary data-interview method-collection of secondary data

**Unit - III**

Thesis or assignment writing – Steps involved in thesis or assignment writing - preliminaries, the text and end matter.

Report writing - significance of report writing-different steps in writing report - sections of a research reports-title page, abstract, table of contents, introduction, body, recommendations, references and appendixes.

**Unit -IV**

Writing a research proposal - introduction, literature review, methodology, expected results, budget and references.

Preparing grant proposal for a research project-content of the summary, introduction to the organisation, statement of the problem, aims and objectives of the project, design of the project-evaluation of the project, future funding, budget proposal.

**Unit -V**

Panel discussion - purpose, objectives, characteristics, advantages and limitations.

General meetings, workshops and seminars: conduct scientific session, the leader, selection of a topic for presentation

**REFERENCE BOOKS:**

1. Thesis and Assignment Writing – J Anderson, B.H. Dursten and M. Poole, Wiley Eastern (1977).
2. Statistical Method, Gupta S. P, Sultan Chand and Sons, New Delhi, 2004
3. Hand Book For Authors –Journal of the American Chemical Society Publications

## **SEMESTER – III**

### **CORE PAPER IX INORGANIC CHEMISTRY- III INORGANIC PHOTOCHEMISTRY, SPECTROSCOPY AND ORGANOMETALLICS**

#### **Objectives**

- ❖ To learn the photo electron spectroscopy of inorganic compounds.
- ❖ To study the theory, determination of structure, growth of crystals.
- ❖ To study the applications of IR, Raman and NMR spectroscopy in inorganic compounds
- ❖ To learn the detail study of synthetic organometallic complexes and their reactivity.
- ❖ To know about ESR and Mössbauer spectroscopy

#### **Expected outcomes**

At the end of the course the learners should able to

- ✓ Use photo electron spectroscopy to inorganic compounds.
- ✓ Predict the crystal structure.
- ✓ Apply and interpret the IR, Raman and NMR spectroscopic data of simple inorganic compounds.
- ✓ Synthesize the organometallic complexes which are very useful in the modern era.
- ✓ Use ESR and Mössbauer spectroscopy to characterise inorganic and organometallic compounds.

#### **UNIT-I INORGANIC PHOTOCHEMISTRY AND PHOTOELECTRONSPECTROSCOPY**

Unimolecular charge-transfer photochemistry of cobalt(III) complexes – mechanism of CTM, photoreduction – ligand-field photochemistry of chromium(III) complexes – Adamson's rules, photoactive excited states, V-C model – photophysics and photochemistry of ruthenium – polypyridine complexes, emission and redox properties. Photoelectron Spectroscopy

PES - Theory, Types, origin of fine structures - shapes of vibrational fine structures – adiabatic and vertical transitions, PES of homonuclear diatomic molecules ( N<sub>2</sub>, O<sub>2</sub>) and heteronuclear diatomic molecules (CO, HCl) and polyatomic molecules (H<sub>2</sub>O, CO<sub>2</sub>, CH<sub>4</sub>, NH<sub>3</sub>) – evaluation of vibrational constants of the above molecules, Koopman's theorem-applications and limitations.

#### **UNIT-II: NUCLEAR AND RADIATION CHEMISTRY**

Properties of nucleus – different types of nuclear forces , Nuclear structure and nuclear stability, Nuclear models- – liquid drop model, shell model of nucleus, Radioactivity and nuclear reactions, nuclear reactions induced by charged particles – Q value – nuclear reaction cross section, significance and determination – theory of nuclear fission, nuclear

fusion, stellar energy. Hot atom chemistry, Nuclear fission and fusion reactors. The interaction of nuclear radiations with matter. Radiation hazards and therapeutics. Detectors and their principles. Tracer Application of radioisotopes in agriculture, industry and medicine. Isotope dilution and radio-activation methods of analysis.

### **UNIT-III: APPLICATIONS OF IR, RAMAN AND NMR SPECTROSCOPY TO INORGANIC COMPOUNDS**

**IR spectroscopy**-Introduction, selection rules, stretching frequency of some inorganic ions- effect of coordination on the stretching frequency- sulphato, carbonato, sulphito, aqua, nitro, thiocyanato, cyano, thiourea, DMSO complexes.

**Raman spectroscopy** –Introduction, combined applications of IR and Raman spectroscopy in the structural elucidation of  $\text{N}_2\text{O}$ ,  $\text{ClF}_3$ ,  $\text{NO}_3^-$ ,  $\text{ClO}_4$ , metal carbonyls.

**NMR spectroscopy**- Introduction, structural assessment of simple inorganic compounds, applications of  $^1\text{H}$ ,  $^{15}\text{N}$ ,  $^{19}\text{F}$ ,  $^{31}\text{P}$ -NMR spectroscopy in structural problems, fluxional molecules, quadrupolar nuclei- effect in NMR spectroscopy, shift reagents- applications.

### **UNIT-IV: ESR AND MÖSSBAUER SPECTROSCOPY**

**ESR spectroscopy**-Introduction, presentation of esr spectra g and A parameters, spin densities, Mc-Connel relationship, factors affecting the magnitude of g and A. Zero field splitting, Kramer's degeneracy, esr spectra of V(II), Mn(II) Fe (II), Co (II), Ni(II), Cu (II) complexes, bis(salicylaldimine)copper (II) ,  $[(\text{NH}_3)_5\text{Co}-\text{O}_2-\text{Co}(\text{NH}_3)_5]^{5+}$ .

**Mössbauer spectroscopy** –Introduction, principle, instrumentation, recoil energy, Doppler effect, number of MB signals, isomer shift, quadrupole splitting, magnetic hyperfine splitting- applications to  $^{57}\text{Fe}$ ,  $^{119}\text{Sn}$  and  $^{129}\text{I}$  compounds.

### **UNIT-V: ORGANOMETALLIC CHEMISTRY**

Types of organometallic compounds on the basis of the nature of M-C bond. EAN rule: 18e- and 16e- rules – determinant of oxidation state, configuration, coordination number of the metal centre – Types and application 18e<sup>-</sup> / 16e<sup>-</sup> rules. Carbonyls – isolated concept.- Structure of carbonyls (simple and polynuclear) Nitrosyls – bridging and terminal nitrosyls, bent and linear nitrosyls. Dinitrogen compounds donors – Alkyl and Aryl – preparation and properties; chain carbon donors – olefins, acetylene and allyl complexes – synthesis, structure and bonding; cyclic carbon donors – (metallocene) – synthesis, structure and bonding.

Important types of reactions of organometallic compounds – substitution – electrophilic and nucleophilic attack on ligands; carbonylation and decarbonylation; oxidative addition and reductive elimination, insertion and deinsertion(elimination). Template synthesis of macrocyclic ligands.

### **Reference and text books**

1. H. Kaur – “Spectroscopy”, 3rd Ed., Pragati Prakasan Publications, Meerut, **2006**.
2. R.S. Drago, Physical methods in inorganic chemistry; Affiliated East-West Press Pvt. Ltd., New Delhi,**2012**.
3. 4. P.J.Wheatley, The determination of molecular structure, 2<sup>nd</sup> edition, Dover Publications, Mineola,**1981**.
5. C.N. Banwell, Fundamentals of molecular spectroscopy 4<sup>th</sup> edition, McGraw Hill Education, Noida,**1994**.
6. H. J. Arniker, Essentials of Nuclear Chemistry, 2<sup>nd</sup> Ed, Wiley Eastern Co, **1987**.
7. G. Friedlander, J. W. Kennedy and J. M. Miller, Nuclear and Radiochemistry, Wiley, **1964**.

## **CORE PAPER X ORGANIC CHEMISTRY - III**

### **SPECTROSCOPY, SPECTROMETRY AND THEIR APPLICATIONS**

#### **Objectives**

- ❖ To understand the basic aspects of NMR spectroscopy and NMR spectra of simple organic molecules.
- ❖ To understand, UV and IR spectra of organic compounds.
- ❖ To understand mass spectral cleavage pattern of organic compounds.
- ❖ To understand the structural elucidation of organic compounds using UV, IR, NMR and Mass Spectral data.

#### **Expected outcomes**

- ✓ To enable the students to correlate the UV absorption values as well as IR stretching frequencies of organic compounds with their functional groups.
- ✓ To enable the students to interpret the  $^1\text{H}$  as well as  $^{13}\text{C}$  NMR spectra of organic compounds with individual nuclei (protons/carbons).
- ✓ To enable the students to understand NMR spectral techniques such as decoupling, NOE and MRI.
- ✓ To enable the students to interpret different types of carbons ( $\text{CH}$ ,  $\text{CH}_2$ ,  $\text{CH}_3$  and quaternary C) using  $^{13}\text{C}$  NMR spectral editing and  $^{13}\text{C}$  NMR DEPT techniques.
- ✓ To enable the students to interpret 2D-NMR techniques such as HSQC, HMBC and NOESY.
- ✓ To enable the students to determine the structure of simple organic compounds from UV, IR, NMR and Mass spectral data.

#### **Unit I: UV AND IR SPECTRA OF ORGANIC COMPOUNDS**

**Electronic absorption:** Beer-Lamberts law, Types of electronic excitation. Chromophore and Auxochrome-Bathochromic and Hypsochromic shift. UV-vis spectra of simple organic compounds such as alkenes, phenols, anilines, carbonyl compounds and 1,3-diketones. Woodward-Fieser rule.

**Infrared Spectra:** Identification of functional groups in Organic Compounds, Finger print region. Inter and Intramolecular hydrogen bonding. Various factors affecting IR stretching frequencies.

#### **Unit II: NUCLEAR MAGNETIC RESONANCE AND THEIR APPLICATIONS**

Origin of NMR spectrum-Nuclear spin states-NMR active nuclei-Nuclear magnetic moment-Larmor equation-Absorption of energy and Resonance-Population density of nuclear spin states. Saturation phenomena-Relaxation mechanisms, Bloch equation (only significance and derivation not required). Comparison of CW and FT instrument-Chemical



shift-Standards in NMR—Shielding and Deshielding—Factors affecting chemical shift—electronegativity, hybridization, hydrogen bonding-anisotropic effect—double bond, triple bond, aromatic compounds, carbonyl compounds and annulenes. Spin-spin coupling—splitting origin and rules—factors affecting coupling constant: cis, trans, gem, ortho, meta, para coupling—exchange with deuterium. Vicinity of the proton, Long range coupling, Karplus equation and curve. Two interacting nuclei: AB, AX, AA'BB', dd, pair of doublet and AB quartet. Three interacting nuclei: AMX, ABX, ABC systems (only pattern is required). Dynamic NMR of DMF, cyclohexane and iodocyclohexane). Double irradiation/Spin decoupling, Nuclear Overhauser Effect (NOE) and NMR imaging (MRI).

### **UNIT-III: $^{13}\text{C}$ NMR, $^{19}\text{F}$ NMR & $^{31}\text{P}$ NMR AND 2-D NMR TECHNIQUES**

$^{13}\text{C}$  NMR—difficulties in recording  $^{13}\text{C}$  NMR: Homo nuclear and heteronuclear coupling. Off Resonance decoupled spectrum identification of various types of carbon (functional groups) using  $^{13}\text{C}$  NMR. Origin of  $^{13}\text{C}$  satellite peaks. Attached Proton Test (APT) & Distortionless Enhancement by Polarization Transfer (DEPT) spectrum (DEPT-45, DEPT-90 and DEPT-135).  $^{19}\text{F}$  NMR—Precessional frequency and heteronuclear coupling. Identification of organofluoro compounds ( $\text{CF}_3\text{CO}_2\text{Et}$  and  $\text{CF}_3\text{CH}_2\text{OH}$ ) using NMR.  $^{31}\text{P}$  NMR— Chemical shift and heteronuclear coupling. Identification of organo phosphorous compounds such as  $(\text{Me})_3\text{P}$ ,  $(\text{EtO})_3\text{P}=\text{O}$  and  $\text{Ph}_3\text{P}$ . P-P bond in NMR.

Basic aspects of 2-D NMR techniques: Correlation spectroscopy (COSY). HOMO COSY (HOMCORR:  $^1\text{H}$ - $^1\text{H}$  connectivity,  $^{13}\text{C}$ - $^{13}\text{C}$  connectivity): HSQC and HETERO COSY (HETCORR): HMBC. 2D NOE Correlation Spectroscopy (NOESY).

### **UNIT-IV: MASS SPECTROMETRY**

Origin, basics and bloc diagram of Mass spectrum-Variou types of Ionization techniques-Stability of Molecular ions, Meta stable ions. Base peaks and Isotope peaks. Fragmentation patterns of organic molecules such as benzenes, phenyl halides, phenols, benzyl alcohols, benzyl halides, aliphatic alcohols, aliphatic as well as aromatic aldehydes, ketones, acids, esters and amides. Fragmentation patterns of aliphatic/aromatic nitro and amine compounds. Fragmentation patterns of heterocyclic compounds (furan, pyrrole and pyridine only). McLafferty rearrangements of organic molecules.

## **UNIT-V: IDENTIFICATION OF ORGANIC COMPOUNDS USING ANALYTICAL AND SPECTRAL DATA**

Determination of molecular formula of organic compounds using elemental (CHN) analysis data. Structural determination of simple organic compounds using UV, IR, NMR and Mass spectral data.

### **Reference and text books**

1. William Kemp, Organic Spectroscopy, Macmillan Education UK, 3<sup>rd</sup> Ed, **1991**.
2. P.S. Kalsi, Spectroscopy of Organic Compounds, New Age International Publishers, 6<sup>th</sup> Ed, Reprint, **2005**.
3. R. M. Silverstein, G. C. Bassler and T. C. Morrill, Spectrometric identification of Organic compounds, John Wiley, 5<sup>th</sup> Ed, **1991**.
4. R. M. Silverstein, F. X. Webster and D. Kiemle, Spectrometric identification of Organic compounds, Wiley, 7<sup>th</sup> Ed, **2005**.
5. William Kemp, NMR in Chemistry: A Multinuclear Introduction, MacMillan, **1988**.
6. R. S. Macomber, A Complete Introduction to NMR Spectroscopy, Wiley, **1998**.
7. Jag Mohan, Organic Spectroscopy Principles & Applications, Alpha Science International Ltd, 2<sup>nd</sup> Ed, **2004**.

## **CORE PAPER XI PHYSICAL CHEMISTRY - III**

### **THERMODYNAMICS AND GROUP THEORY**

#### **Objectives**

- ❖ *To know the limitations of classical thermodynamics in the evaluation of macroscopic properties.*
- ❖ *To understand the principles of activity and fugacity.*
- ❖ *To know the theories of kinetic activity.*
- ❖ *To study the techniques of Heat Capacity.*
- ❖ *To learn about the various applications of Quantum Statistics.*
- ❖ *To understand the concepts of group theory*
- ❖ *To apply group theory for determining vibrations, hybrid orbitals*
- ❖ *To determine the selection rules for spectral transitions, energies and molecular orbitals*

#### **Expected outcomes**

- ✓ *Know the limitations of classical thermodynamics in the evaluation of macroscopic properties.*
- ✓ *Understand the principles of activity and fugacity.*
- ✓ *Know the theories of kinetic activity.*
- ✓ *Understand the techniques of Heat Capacity.*
- ✓ *learn about the various applications of Quantum Statistics.*
- ✓ *Understand the rules and concepts of group theory*
- ✓ *To apply group theory for determining vibrations and hybrid orbitals*
- ✓ *To determine the selection rules for spectral transitions, energies and molecular orbitals*

#### **UNIT-I: THERMODYNAMICS AND NON-IDEAL SYSTEMS**

Concepts of Partial Molar Properties-Partial Molar Free Energy and Partial Molar Volume. Gibbs-Duhem equation, Chemical potential-Variation of chemical potential with temperature and pressure, Van't Hoff isotherm.

#### **UNIT-II: IRREVERSIBLE THERMODYNAMICS**

Nernst heat theorem-Third law of thermodynamics-Applications of third law-Entropy change-Calculation of absolute entropies-Apparent exceptions to third law- Non-equilibrium thermodynamics-Basic concepts-Forces and fluxes-Entropy of irreversible processes-Entropy production-Clausius inequality-Phenomenological equations-Onsager reciprocity relations-Coupled reactions. The principle of microscopic reversibility, the Onsager reciprocal relations – verification. Entropy production- rate of entropy production, entropy production in chemical reactions.

### **UNIT-III: STATISTICAL THERMODYNAMICS I**

Objectives of statistical thermodynamics, Concept of distributions, Types of ensembles. Thermodynamic probability, Most probable distribution Law- Classical statistics-Maxwell-Boltzmann (MB) statistics-Quantum statistics-Bose-Einstein (BE) and Fermi-Dirac (FD) statistics-Derivation of distribution function-MB, BE and FD statistics-comparison-

### **UNIT IV: GROUP THEORY-I**

Symmetry elements; symmetry operations, Abelian group-point groups-determination of point group- Group multiplication table - Matrix representation of symmetry operations-Similarity transformations; Space groups of crystals-Mulliken symbols-reducible and irreducible representations; Symbols and rules of irreducible representations-reduction formula-direct product representation; Great orthogonality theorem; character table-construction of character tables  $C_{2v}$ ,  $C_{3v}$  and  $D_{2h}$ .

### **UNIT V: PHOTOCHEMISTRY**

Jablonski diagram, Primary and Secondary Processes, quantum yield and its determination-chemical actinometer. Excimers and exciplexes-Kinetics of collisional quenching-Stern Volmer equations. Photosensitization, Chemiluminescence. Photosynthesis, solar energy conversions. Semiconductor photo catalysis, lasers.

Radiation Chemistry-linear energy transfer, G-value, dosimeters, radiolysis of water, solvated electrons.

### **Reference and text books**

1. A. Walton, Molecular and Crystal Structure Models, Ellis Horwood, Chichester, **1978**.
2. A. R. West, Solid State Chemistry and its applications, John Wiley and Sons, New York, **1984**.
3. M. C. Gupta, Statistical Thermodynamics, Wiley Eastern, New Delhi, **1990**.
4. J. Rajaram and J. C. Kuriacose, Irreversible Thermodynamics, Lal Nagin Chand, New Delhi, **1989**.
5. P. W. Atkins, Physical Chemistry, Oxford University Press, Oxford, **1990**.
6. D. A. McQuarrie, Text Book of Physical Chemistry, University Science Books, Mill Valley, California, **1983**.
7. V. Ramakrishnan and M. S. Gopinathan, Group theory in Chemistry, Vishal Publications, **1988**.
8. J. Rajaram and J. C. Kuriacose, Thermodynamics for Students of Chemistry, Lal Nagin Chand, New Delhi, **1986**.
9. F.A. Cotton, Chemical Application of Group Theory, John Wiley and Sons Inc. New York, **1971**.
10. K.V. Raman, Group theory and its applications to Chemistry, Tata McGraw-Hill Publishing Company, **1990**.

**Core Paper XII - Practical-III    Subject code**  
**INORGANIC CHEMISTRY PRACTICAL**

1. Preparation of Inorganic Complexes – Sodium hexanitrocobaltate (III), Chloropentamminecobalt (III) Chloride, bis (acetyl acetonato) Copper (II), Hexamminenickel (II) chloride. Tris copper thiourea, Copper (I) chloride Trinitro triammine Cobalt (III) Sodium cuprous tiosulphate.
2. Titrimetry and Gravimetry:
  - i. Estimation of copper and zinc present in a mixture, copper – Volumetrically Zinc Gravimetrically/Complexometrically.
  - ii. Estimation of copper and nickel present in a solution copper - Volumetrically nickel Gravimetrically/Complexometrically.
  - iii. Estimation of Calcium and Magnesium Calcium – Volumetrically Magnesium Complexometrically
  - iv. Estimation of Mg and Ni both complexometrically.
3. Applied Analysis
  - i. Analysis of any two of the following alloys – Brass, Bronze, Solder, Stainless steel.
  - ii. Analysis of any two of the following minerals – Dolomite, Pyreusite and Zinc blends.
4. Interpretation of spectra (IR, UV, Mossbauer, NQR etc.,)

## **ELECTIVE III**

### **MATERIAL CHEMISTRY**

#### **Objectives**

- ❖ To learn the synthesis and characterization techniques of nanomaterials.
- ❖ To learn the theories of conducting properties of materials.
- ❖ To learn the structural importance of industrially important materials.
- ❖ To acquire the knowledge about polymers, types of polymers, Mechanism and Kinetics of polymerization.
- ❖ To understand the Principles of Polymer reactivity and stereochemistry of Polymerization.
- ❖ To get deep knowledge about various methods of polymerization and specialty Polymers.

#### **Expected outcomes**

- ✓ Understand the synthesis and characterization techniques of nanomaterials.
- ✓ Understand the theories of conducting properties of materials.
- ✓ Get the knowledge on the structural importance of industrially important materials.
- ✓ Acquire the Knowledge about polymers, types of polymers, Mechanism and Kinetics of polymerization.
- ✓ Understand the Principles of Polymer reactivity and stereochemistry of Polymerization.
- ✓ Get deep knowledge about various methods of polymerization and specialty Polymers.

#### **UNIT - I: SYNTHESIS AND APPLICATIONS OF NANOMATERIALS**

Preparation of nanomaterials – plasma arcing, CVD, electrodeposition, sol-gel synthesis, ball milling, uses of natural nanoparticles. Synthesis and applications of carbon nanotubes

Self assembled monolayers – monolayers on gold – preparation – structure – growth process – patterning mono layers – mixed mono layers.

Semiconductor quantum dots – synthesis – electronic structure & spectral properties

Monolayer-protected metal nanoparticles – characterization – functionalization – Application - Core-Shell nanoparticles – introduction – types of systems – characterization – properties – Applications of Nanosensors – electrochemical sensors, sensors based on physical properties – nanobiosensors.

#### **UNIT - II: CHARACTERIZATION OF NANOMATERIALS**

Electron microscopes – scanning electron microscopy (SEM), Transmission electron microscopy (TEM), Scanning Transmission Electron Microscopy (STEM), Scanning Probe Microscopy (SPM) – scanning tunneling microscopy (STM) – Atomic manipulations, Focused Ion beam (FIB) technique – Atomic force microscopy (AFM) – scanning probe

Lithography (SPL), Dip pen nanolithography (DPN) - Optical microscopies for nanoscience and Technology – Confocal microscopy – scanning near-field optical microscopy – particle size analysis.

### **UNIT III: POLYMERS**

Polymers - definition - types of polymers - liquid crystalline polymers. Molecular mass - number and mass average molecular mass - determination of molecular mass (osmometry, viscosity, diffusion, light scattering, and sedimentation methods). viscoelasticity, Rubber elasticity. Kinetics of linear stepwise polymerization - addition polymerization - free radical, cationic and anionic polymerization. Kinetics of copolymerization. Polymerization in homogeneous and heterogeneous systems - stereochemistry and mechanism of polymerization. Coordination Polymerization: Kinetics; mono and bimetallic mechanism.

### **UNIT IV: PROCESSING AND PROPERTIES OF POLYMERS**

Polymer Processing: Plastics elastomers and fibres. Compounding processing techniques: calendaring, die casting, rotational casting, film casting, injection moulding, blow moulding extrusion moulding, thermoforming, foaming, reinforcing and fibre spinning. Polymer structure and physical properties – crystalline melting point  $T_m$ . Determination of  $T_g$ . Relationship between  $T_m$  and  $T_g$ .

### **UNIT V: COMMERCIAL POLYMERS**

Polyethylene, polyvinyl chloride, polyamides, polyesters, phenolic resins, epoxy resins and silicone polymers. Functional polymers-Fire retarding polymers and electrically conducting polymers. Biomedical polymers.

### **References and text books**

1. R. Alcock and F. W. Lamber, Contemporary Polymer Chemistry, Prentice Hall, **1981**.
2. G. Hodes (Eds.), Electrochemistry of Nanomaterials, Wiley-VCH, **2001**.
3. R. J. Young and P. A. Lovell, Introduction to Polymers, 2<sup>nd</sup> Ed, Chapman and Hall, **2002**.
4. V. R. Gowariker, N. V. Viswanathan and Jayadev Sreedhar, New Age International (P) Ltd, **2005**.
5. F. W. Billmeyer, Text Book of Polymer Science, 3<sup>rd</sup> Ed, John Wiley & Sons, New York, **2003**.
6. C. N. R. Rao, A. Muller and A. K. Cheetham (Eds.), The Chemistry of Nanomaterials Vol.I & Vol.II, Wiley-VCH, **2004**.

## **Elective PAPER- V**

### **BIO CHEMISTRY**

#### **OBJECTIVES:**

*This course aims to explain the basic concepts in Chemistry and Metabolism of Carbohydrates, amino acids, Proteins and Lipids. In addition to this, the student can gain the full understanding of various types of Nucleic acids and classification of Vitamins and Enzyme.*

#### **UNIT I - CHEMISTRY AND METABOLISM OF CARBOHYDRATES**

Definition, classification and biological role of carbohydrates      Monosaccharide  
Linear and ring structures (Haworth formula) of ribose, glucose, fructose and mannose  
(structural determination not required) physical and chemical properties of glucose and fructose.

Disaccharides: Ring structures (Haworth formula) - occurrence, physical and chemical properties of maltose, lactose and sucrose.

Polysaccharides: Starch, glycogen and cellulose - structure and properties.  
Glycolysis of carbohydrates.

#### **UNIT II - CHEMISTRY AND METABOLISM OF AMINO ACIDS AND PROTEINS**

Amino acids: Various classifications, essential amino acids, physical properties (amphoteric nature and isoelectric point) and reactions.

Proteins: Classifications (based on shape, composition and solubility), physical properties. Primary structure - End group analysis (N- terminal analysis- Edman's method, dansyl chloride method; C - terminal analysis- hydrazinolysis and bio - chemical methods)  
Biological functions of proteins, Deamination, transamination reactions, Urea cycle.

#### **UNIT III - CHEMISTRY AND METABOLISM OF LIPIDS:**

Definition, classification- simple lipids (fatty acids), compound lipids and derived lipids. Properties: saponification number, Acetyl number.

Sterols: Cholesterol (structure not needed), biological importance and chemical properties.  
Bile acids- functions. Biological functions of lipids.

#### **UNIT IV - NUCLEIC ACIDS:**

Purine and pyrimidine bases, nucleosides, nucleotides, polynucleotide, DNA structure - various types, RNA structure - various types. Biological functions of DNA and RNA, Genetic code.



## **UNIT V – VITAMINS AND MINERALS:**

Vitamins: Definition, classification- water-soluble vitamins (B<sub>1</sub> B<sub>2</sub>, B<sub>3</sub>, B<sub>6</sub>, B<sub>12</sub> and vitamin-C) and fat-soluble vitamins (A, D, E and K) - occurrence, structure, deficiency diseases, biochemical roles and daily requirements.

Minerals; Ca, P, Na, K and Mg. and trace elements –Fe, Cu and Se

## **SUGGESTED REFERENCE BOOKS:**

1. Biochemistry C.B. Powar and G.R. Chatwal.
2. Elements of Biochemistry Ragunatha Rao
3. Essential Biochemistry U. Sathyanarayanan
4. Essential Biochemistry J.L. JAIN.

## **SEMESTER – IV**

### **CORE XIII ORGANIC CHEMISTRY - IV PHOTOCHEMISTRY, PERICYCLIC REACTIONS, HETEROCYCLES AND NATURAL PRODUCTS**

#### **Objectives**

- ❖ To understand photochemical reactions along with their mechanism and synthetic utility.
- ❖ To understand various types of pericyclic reactions with orbital symmetry based selection rule.
- ❖ To understand the synthesis and reactivity of five- as well as six-member heterocycles.
- ❖ To understand the structural elucidation, biosynthesis and synthesis of natural products.

#### **Expected outcomes**

- ✓ To enable the students to understand reaction mechanisms involved in photochemical and pericyclic reactions.
- ✓ To enable the students to understand synthesis and reactivity of five member and six member heterocycles.
- ✓ To enable the students to understand the isolation, classification, structural elucidation and synthesis of terpenes.
- ✓ To enable the students to understand the structural elucidation and biosynthesis of steroids and alkaloids.

#### **UNIT-I: ORGANIC PHOTOCHEMISTRY**

Principles of Photochemistry and Photochemical reactions: Norrish type I & II reactions. Paterno-Büchi reaction; Photochemistry of enones and dienones: [2 + 2] photochemical cycloaddition; Photo Fries, di- $\pi$  methane, oxa & aza di- $\pi$  methane rearrangements.

#### **UNIT II: ORBITAL SYMMETRY & PERICYCLIC REACTIONS**

Selection rules (Woodward and Hoffmann rules) and stereochemistry of electrocyclic reactions, cycloadditions and Sigmatropic reactions-FMO approach, Correlation diagram approach, Huckel-Mobius approach and perturbation molecular orbital approach.

#### **UNIT-III: HETEROCYCLES AND THEIR REACTIVITY**

Structure, synthesis and their reaction of the following systems; a) One heteroatom - Pyrrole, Furan, Thiophene, Pyridine; b) Benzo fused Heterocycles - Indole, Quinoline; c) Two heteroatom - Pyrazole, Imidazole, Pyrimidine, Pyrazine.

#### **UNIT-IV: NATURAL PRODUCTS: TERPENOIDS & STEROIDS**

**Terpenoids:** Isolation and classification - general methods to elucidate the structure of terpenoids - methods of structure elucidation and synthesis as applied to zingiberine - eudesmol - caryophyllene - abietic acid - santonin - biosynthesis of terpenes.

**Steroids:** Structural elucidation of cholesterol – ergosterol- vitamin-D – equilenin – estrone - progesterone, Stigmasterol, Steroid hormones, androsterone, testosterone, biosynthesis of steroids – Structure - Synthesis of bile acids.

#### **UNIT-V: NATURAL PRODUCTS: ALKALOIDS**

Structural elucidation and biosynthesis of dictamnine–chinconine–morphine – reserpine – aeronycline – cocaine – lysergic acid and nicotine.

#### **Reference and text books**

1. R. K. Bansal, Heterocyclic Chemistry, New Age International (P) Ltd, 5<sup>th</sup> Ed, **2014**.
2. Charles A. Depuy and Orville L. Chapman, Englewood Cliffs, Molecular reactions and Photochemistry, New Jersey: Prentice-Hall, **1972**.
3. Nicholas J Turro, V. Ramamurthy and J. C. Scaiano, Modern Molecular Photochemistry for Organic Molecules, University Science Books, 1<sup>st</sup> Ed, **2010**.
4. Jagdamba Singh and Jaya Singh, Photochemistry and Pericyclic Reactions, New Age International (P) Ltd, 3<sup>rd</sup> Ed, **2012**.
5. P. L. Gilchrist and R. C. Storr, Organic Reactions & Orbital Symmetry, Cambridge [Eng.] University Press, **1972**.
6. I. L. Finar, Organic Chemistry Vol 1 & 2, Dorling Kindersley India (P) Ltd, **2009**.
7. A. Newman, Chemistry of Terpenes and Terpenoids, Academic Press, **1972**.

**Core Paper-XV - Practical-III Subject code**  
**PHYSICAL CHEMISTRY & ORGANIC CHEMISTRY PRACTICAL**

**PHYSICAL CHEMISTRY PRACTICAL:**

**KINETICS:**

1. Determination of Arrhenius parameters.
2. Study of primary salt effect.
3. Determination of order of a reaction spectrophotometrically.
4. Study of inversion of cane sugar polarimetrically.

**CONDUCTOMETRY:**

5. Determination of strength of strong acid and weak acid present in a mixture.
6. Study of saponification of ethylacetate conductometrically.

**POTENTIOMETRY:**

7. Determination of strength KCl and KI present in a mixture potentiometrically.
8. Determination of solubility product of silver halide by chemical cell and concentration cell methods.

**SPECTRAL INTERPRETATION:**

9. NMR, IR, UV, ESR

**ORGANIC CHEMISTRY PRACTICAL:**

Organic preparations involving two or three stages, quantitative estimation of organic compounds using known methods, basic training for extraction of compounds from natural products and then chromatographic separations.

**I. ANY SIX PREPARATIONS FROM THE FOLLOWING INVOLVING TWO STAGES:**

1. Sym-Tribromobenzene from aniline.
2. p-nitro aniline from acetanilide
3. m-Nitrobenzoic acid from methyl benzoate.
4. 2, 4-Dinitrobenzoic acid from p-nitro toluene.
5. m-Nitro benzoic acid from benzaldehyde
6. p-bromoaniline from acetanilide
7. Anthraquinone from phthalic anhydride.
8. Phthalide from phthalic anhydride
9. 2-phenyl indole from phenylhydrazine
10. 2,4- Dinitrophenyl hydrazine from p-nitrochlorobenzene.

**II. ANY FIVE ESTIMATIONS:**

1. Estimation of aniline
2. Estimation of phenol
3. Estimation of glucose (Bertrands Methods)
4. Saponification of fat or an oil.

5. Iodine value of an oil.
6. Estimation of Ketone.
7. Estimation of amino group.
8. Estimation of amide group
9. Estimation of sulphur in an organic compound.

**III. ANY TWO EXERCISES IN THE EXTRACTION OF NATURAL PRODUCTS:**

1. Caffeine from tea leaves
2. Lactose from milk
3. Citric acid from lemon
4. Piperine from black pepper

**IV. CROMATOGRAPHIC SEPARATIONS:**

1. Column chromatography - separation of anthracene and acid from anthracene picrate.
2. Thin layer chromatography separation of green leaf pigments.
3. Paper chromatography
- 4 Identification of amino acids.

**V. SPECTRAL INTERPRETATION OF ORGANIC COMPOUNDS.  
UV, IR, PMR AND MASS SPECTRA OF ANY TEN COMPOUNDS.**

1. 1, 3, 5-Trimethylbenzene
2. Pinacolone
3. propyl amine
4. p-Methoxybenzyl alcohol
5. Benzyl bromide
6. Phenyl acetone
7. 2-Methoxyethyl acetate
8. Acetone
9. Isopropyl alcohol
10. Acetaldehyde diacetate
11. N, N-Dimethylamino ethanol
12. Pyridine
13. 4-Picoline
14. 1, 3 dibromo-1, 1-dichloropropene
15. Cinnamaldehyde

**CORE PAPER XIV PHYSICAL CHEMISTRY - IV**  
**STATISTICAL THERMODYNAMICS, GROUP THEORY AND**  
**SURFACE TECHNIQUES**

**UNIT I THERMODYNAMICS II**

Fugacity–Determination of fugacity of gases by graphical method-Variation of fugacity with temperature and pressure -Lewis Randal rule-Duhem-Margules equation. Determination of activity and activity coefficient of non-electrolyte (e.m.f method)-Excess functions.

**UNIT II IRREVERSIBLE THERMODYNAMICS II**

Phenomenological equations-Onsager reciprocity relations-Coupled reactions.The principal of microscopic reversibility, the Onsager reciprocal relations – verification.Entropy production- rate of entropy production, entropy production in chemical reactions.

**UNIT III STATISTICAL THERMODYNAMICS II**

Partition functions-Translational, rotational, vibrational and electronic partition function –Calculation of thermodynamic parameters and equilibrium constants in terms of partition function; Debye and Einstein heat capacity of solids.

**UNIT IV GROUP THEORY-II**

Applications of group theory- Determination of representations of vibrational modes in non-linear molecules such as water, ammonia,  $\text{BF}_3$ ,  $\text{CH}_4$  and  $\text{XeF}_4$ .Determination of Hybrid orbitals in non-linear molecules – Examples:  $\text{H}_2\text{O}$ ,  $\text{NH}_3$ ,  $\text{BF}_3$ ,  $\text{CH}_4$  and  $\text{XeF}_4$ . SALC procedure-evaluation of energies and molecular orbitals for systems like ethylene and butadiene.Selection rules for spectral transitions. Electronic spectra of formaldehyde and ethylene.

**UNIT V SURFACE AND THERMAL ANALYSIS TECHNIQUES**

Principles, theory, instrumentation and applications of SEM, STM, TEM, AFM, ESCA -interpretation of spectra-Merits and demerits.

Principles, theory and applications of TGA, DTA, DSC, DTG. Interpretation of various thermal analysis curves.

**References**

1. Yi-Chen Cheng, Macroscopic and Statistical Thermodynamics, World Scientific, **2006**.
2. S. Glasstone, Thermodynamics for Chemists, Affiliated East West Press, New Delhi, **1960**.
3. V. Ramakrishnan and M. S. Gopinathan, Group theory in Chemistry, Vishal Publications, **1988**.
4. K.V. Raman, Group theory and its applications to Chemistry, Tata McGraw-Hill Publishing Company, **1990**.

## **Elective Paper – IV**

### **BIOINORGANIC CHEMISTRY**

#### **UNIT I**

Inorganic elements in biological systems, Basic Bioenergetics and classification of enzymes. Active transport of cations across membranes, Sodium pump, Biology of calcium carriers and the role in muscle contraction. Enzyme stabilisation, clotting of blood and biological calcification.

#### **UNIT II**

Porphyrin ring system – metalloporphyrins – hemoglobin and myoglobin – structures and work functions – synthetic oxygen carriers – cytochromes – structure and work functions – in respiration – chlorophyll – structure – photosynthetic sequence – iron-sulphur proteins (non-heme iron protein).

#### **UNIT III**

Metal ion deficiency and disease: Fe, Cu and Zn. Metal ion toxicity: Classes of toxic metal compounds – Cu, Cd, Fe, Pb, Ca and Hg toxicity – detoxification. Molecular mechanism of ion transport across the membrane – sodium and potassium ions pumps.

#### **UNIT IV**

Metals in medicine: Au in rheumatic arthritis – Pt, Au and metallocenes in anticancer drugs – metals in radio diagnosis and magnetic resonance imaging. Biological cycles: Nitrogen cycle – hydrogen cycle.

#### **UNIT V**

Metal storage and transport: Fe, Cu, Zn and V storage and transport – metallothioneins: transporting some toxic metals –  $\text{Zn}^{2+}$  ion complexes: carbonic anhydrase II – carboxypeptidase A, Carboxypeptidase G2, Cobalt for Zn ion substitution.

#### **Text Books**

1. S.J.Lippard & J.M.Berg. Principles of Bioinorganic Chemistry, Panima Publ.Corp.(2005)
2. E.I.Ochiai. Bioinorganic Chemistry –An Introduction, Allyn and Baccon Inc.(1977)
3. M.N.Huhes . The Inorganic Chemistry of Biological Processes, Wiley (1981)
4. R.P.Hanzlik. Inorganic Aspects of Biological and Organic Chemistry, Academic Press(1976)
5. H.Kraatz & N.Metzler – Nolte (Eds). Concept and Models in Bioinorganic Chemistry, Wiley(2006)
6. I.Bertini, H.B.Gray, S.J.Dippard & J.S.Valentine, Bioinorganic Chemistry, Viva Books Pvt.Ltd.(2004)

## **Extra Disciplinary Elective Paper – II**

### **ENVIRONMENTAL CHEMISTRY**

#### **Unit I: Energy and Environment**

Sources of energy: Renewable energy sources – solar energy –solar –water heating system-solar energy flow through ecosystem-hydro energy-tidal energy-wind energy-biomass energy-production of biogas-geothermal energy. Non-renewable energy sources-types of coal-pollution caused by coal-Petroleum - refining of petroleum by fractional distillation-products of fractional distillation-natural gas-natural gas as energy source-pollution caused by burning fossil fuels-Nuclear energy.

#### **Unit II: Air Pollution**

Major air pollutants-oxides of carbon, oxides of nitrogen, oxides of sulphur, particulates –sources and effects –smog and photochemical smog-sources of air pollution-Effects of air pollution-acid rain-green house effect-global warming-depletion of ozone-control of air pollution – Instrumental methods of measuring air pollution-HPLC and X-ray fluorescence spectroscopy.

#### **Unit III: Soil Pollution and Noise Pollution**

**Soil Pollution:** Sources of soil pollution-industrial pollution-urban and domestic wastes-radioactive pollutants-agrochemicals: Fertilizers-salination of soils-pesticides-insecticides: organochlorines, organophosphates, carbamates and pyrethroids-effects of insecticides on environment – Fungicides and herbicides-types and effects of fungicides and herbicides on environment - plastic and polymers-effect of polymers and plastics on environment –waste treatment .

**Noise Pollution:** sources and effects of noise pollution-control of noise pollution.

#### **Unit IV: Environmental Pollution and Health**

Effect of air pollution on human health-water pollution and health-effect of soil pollution on human health-pollutants encountered at homes(indoor pollution)-pollutants encountered at work place.

#### **Unit V: Environmental Toxicology**



Chemicals in the environment: toxic chemicals in air-toxic elements in water-toxic waste in solids-biodegradability-principles of biodegradation-microbial transformation: biooxidations-bioreductions-and biohydrolysis-impact of toxic chemicals on enzymes:biochemical effects of arsenic, cadmium, lead, mercury and carcinogens-some environmental episodes: Bhopal gas tragedy-chernobyl disaster, three mile island disaster and minamata disaster-better industrial process: green chemistry – designing a green synthesis.

Text Books:

1. Environmental Chemistry by V.K. Ahluwalia, Ane Book Pvt. Ltd.

