DEPARTMENT OF CHEMISTRY

Curriculum and Syllabus for Postgraduate Programme in Chemistry
Under Credit Semester System
(with effect from 2015 admissions)

St. Berchmans College
Affiliated to Mahatma Gandhi University, Kottayam, Kerala
Changanassery, Kottayam, Kerala, India-686101
DEPARTMENT OF CHEMISTRY

Curriculum and Syllabus for
Postgraduate Programme in
Chemistry
Under Credit Semester System
(with effect from 2015 admissions)

St Berchmans College
AUTONOMOUS
College with Potential for Excellence/Reaccredited by NAAC with A Grade
Affiliated to Mahatma Gandhi University, Kottayam, Kerala
Changanassery, Kottayam, Kerala, India-686101
BOARD OF STUDIES

1. **Dr. K C Philip (Chairman)**
   Head & Associate Professor
   Department of Chemistry
   St Berchmans College, Changanassery

2. **Dr. S Sugunan**
   Emeritus Professor
   Department of Applied Chemistry
   Cochin University of Science and Technology

3. **Dr. Sabu Thomas**
   Director
   International & Inter University Centre for Nanoscience & Nanotechnology
   Mahatma Gandhi University
   Kottayam

4. **Dr. Kuruvilla Joseph**
   Head, Department of Chemistry
   Indian Institute of Space Science & Technology
   Thiruvananthapuram

5. **Dr. P Narayanan**
   Scientist
   Indian Rare Earth Ltd.
   Udyogamandal, Ernakulam

6. **Dr. T Muraleedharan Nair**
   Managing Director
   Rubber Development & Training Centre
   Parvanendu, Vidya Nagar
   Perunna P O, Changanassery
7. Dr. Bibin John  
Lithium Ion and Fuel Cell Division  
Vikram Sarabhai Space Centre  
Thiruvananthapuram

8. Dr. Shaji Joseph  
Associate Professor  
Department of Chemistry  
St Berchmans College, Changanassery

9. Dr. P C Thomas  
Associate Professor  
Department of Chemistry  
St Berchmans College, Changanassery

10. Dr. Tomlal Jose E  
Assistant Professor  
Department of Chemistry  
St Berchmans College, Changanassery

11. Dr. Bejoy Francis  
Assistant Professor  
Department of Chemistry  
St Berchmans College, Changanassery

12. Dr. Shijo K Cherian  
Assistant Professor  
Department of Chemistry  
St Berchmans College, Changanassery

13. Dr. Cyril Augustine V  
Assistant Professor  
Department of Chemistry  
St Berchmans College, Changanassery
REGULATIONS FOR POSTGRADUATE PROGRAMME IN CHEMISTRY UNDER CREDIT SEMESTER SYSTEM 2015

1. SHORT TITLE
1.1 These Regulations shall be called St. Berchmans College (Autonomous) Regulations (2015) governing postgraduate programme in Chemistry under the Credit Semester System.
1.2 These Regulations shall come into force with effect from the academic year 2015-2016 onwards.

2. SCOPE
2.1 The regulation provided herein shall apply to postgraduate programme in Chemistry programme, conducted by St. Berchmans College (Autonomous) with effect from the academic year 2015-2016.

3. DEFINITIONS
3.1 ‘University’ means Mahatma Gandhi University, Kottayam, Kerala.
3.2 ‘College’ means St. Berchmans College (Autonomous).
3.3 There shall be an Academic Committee nominated by the Principal to look after the matters relating to the postgraduate programme in Chemistry under the Credit Semester System.
3.4 ‘Academic Council’ means the Committee consisting of members as provided under section 107 of the Autonomy Ordinance, Government of Kerala.
3.5 ‘Parent Department’ means the Department of Chemistry.
3.6 ‘Department Council’ means the body of all teachers of the Department of Chemistry.
3.7 ‘Faculty Mentor’ is a teacher nominated by a Department Council to coordinate the continuous evaluation and other academic activities of the postgraduate programme in Chemistry undertaken in the Department.
3.8 ‘Programme’ means the entire course of study and examinations.
3.9 ‘Duration of Programme’ means the period of time required for the conduct of the programme. The duration of postgraduate programme in Chemistry shall be four (4) semesters.
3.10 ‘Semester’ means a term consisting of a minimum of ninety (90) working days, inclusive of examination, distributed over a minimum of eighteen (18) weeks of five (5) working days each.
3.11 ‘Course’ means a segment of subject matter to be covered in a semester. Each Course is to be designed under lectures/tutorials/seminar/project/practical/assignments/evaluation etc., to meet effective teaching and learning needs.

3.12 ‘Course Teacher’ means the teacher who is taking classes on the course.

3.13 ‘Core Course’ means a course that the student admitted to a particular programme must successfully complete to receive the Degree and which cannot be substituted by any other course.

3.14 ‘Elective Course’ means a course, which can be substituted, by equivalent course from the same subject and the number of courses required to complete the programme shall be decided by the Board of Studies.

3.15 ‘Project’ means a regular project work with stated credits on which the student conducts a project under the supervision of a teacher in the parent department/any appropriate research centre in order to submit a dissertation on the project work as specified.

3.16 ‘Plagiarism’ is the unreferenced use of other authors’ material in dissertations and is a serious academic offence.

3.17 ‘Seminar’ means a lecture expected to train the student in self-study, collection of relevant matter from books and Internet resources, editing, document writing, typing and presentation.

3.18 ‘Tutorial’ means a class to provide an opportunity to interact with students at their individual level to identify the strength and weakness of individual students.

3.19 ‘Evaluation’ means every student shall be evaluated by in-semester assessment (25%) and end-semester assessment (75%).

3.20 ‘Improvement Examination’ is an examination conducted to improve the performance of student in the courses of a particular semester.

3.21 ‘Supplementary Examination’ is an examination conducted for students who fail in the courses of a particular semester.

3.22 ‘Improvement Course’ is a course registered by a student for improving the performance in that particular course.

3.23 ‘Supplementary Course’ is a course that is repeated by a student for having failed in that course in an earlier registration.

3.24 The minimum credits required for completing postgraduate programme in Chemistry is eighty (80).

3.25 ‘Credit’ (C) of a course is a measure of the weekly unit of work assigned for that course in a semester.
3.26 ‘Course Credit’: One credit of the course is defined as a minimum of one (1) hour lecture/minimum of two (2) hours lab/field work per week for eighteen (18) weeks in a semester. The course will be considered as completed only by conducting the final examination.

3.27 ‘Grade’ means a letter symbol (A, B, C etc.) which indicates the broad level of performance of a student in a course/semester/programme.

3.28 ‘Grade Point’ (GP) is the numerical indicator of the percentage of marks awarded to a student in a course.

3.29 ‘Credit Point’ (CP) of a course is the value obtained by multiplying the grade point (GP) by the credit (C) of the course.

3.30 ‘Semester Credit Point Average’ (SCPA) of a semester is calculated by dividing total credit points obtained by the student in a semester by total credits of that semester and shall be rounded off to two decimal places.

3.31 ‘Cumulative Credit Point Average’ (CCPA) is the value obtained by dividing the sum of credit points in all the courses obtained by the student for the entire programme by the total credits of the whole programme and shall be rounded off to two decimal places.

3.32 ‘Weighted Average Score’ means the score obtained by dividing sum of the products of marks secured and credit of each course by the total credits of that semester/programme and shall be rounded off to two decimal places.

3.33 ‘Grace Marks’ means marks awarded to course/courses, in recognition of meritorious achievements of a student in NCC/NSS/Sports/Arts and cultural activities.

4. PROGRAMME STRUCTURE

4.1 Students shall be admitted into the four semester postgraduate programme in Chemistry.

4.2 The programme shall include two types of courses; core courses and elective courses. There shall be a project with dissertation to be undertaken by all students. The programme will also include assignments, seminars, practical, viva-voce etc.

4.3 Total credits for the programme is eighty (80). No course shall have more than four (4) credits.

4.4 Project

Project shall be completed by working outside the regular teaching hours. Project shall be carried out under the supervision of a teacher in the concerned department. A student may, however, in certain cases be permitted to work on the project in an
industrial/research organization on the recommendation of the Supervisor. There shall be an internal assessment and external assessment for the project. The external evaluation of the project work is followed by presentation of work including dissertation and viva-voce.

4.5 **Evaluations**

The evaluation of each course shall contain two parts.

i. Internal or In-Semester Assessment (ISA)

ii. External or End-Semester Assessment (ESA)

Both ISA and ESA shall be carried out using indirect grading. The ISA:ESA ratio is 1:3. Marks for ISA is 25 and ESA is 75 for courses with or without practical.

4.6 **In-semester assessment**

There are four components for ISA, which include attendance, assignment, seminar and in-semester examination.

<table>
<thead>
<tr>
<th>Components of ISA</th>
<th>Marks</th>
</tr>
</thead>
<tbody>
<tr>
<td>Attendance</td>
<td>5</td>
</tr>
<tr>
<td>Assignment</td>
<td>5</td>
</tr>
<tr>
<td>Seminar</td>
<td>5</td>
</tr>
<tr>
<td>In-semester examination(2×5 = 10)</td>
<td>10</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td><strong>25</strong></td>
</tr>
</tbody>
</table>

4.7 Attendance evaluation of students for each course shall be as follows:

<table>
<thead>
<tr>
<th>% of Attendance</th>
<th>Marks</th>
</tr>
</thead>
<tbody>
<tr>
<td>95 and above</td>
<td>5</td>
</tr>
<tr>
<td>90 - 94</td>
<td>4</td>
</tr>
<tr>
<td>85 - 89</td>
<td>3</td>
</tr>
<tr>
<td>80 - 84</td>
<td>2</td>
</tr>
<tr>
<td>75 - 79</td>
<td>1</td>
</tr>
</tbody>
</table>

4.8 **Assignments**

Every student shall submit at least one assignment as an internal component for every course.

4.9 **Seminar**

Every student shall deliver one seminar as an internal component for every course. The seminar is expected to train the student in self-study, collection of relevant matter from the books and internet resources, editing, document writing, typing and presentation.
4.10 **In-semester examination**

Every student shall undergo at least two in-semester examinations as class test as an internal component for every course.

4.11 To ensure transparency of the evaluation process, the ISA mark awarded to the students in each course in a semester shall be published on the notice board according to the schedule in the academic calendar published by the College. There shall not be any chance for improvement for ISA. The faculty mentor shall maintain the academic record of each student registered for the course which shall be forwarded to the office of the Controller of Examinations through the Head of the Department and a copy should be kept in the office of the Head of the Department for at least two years for verification.

4.12 **In-semester assessment of practical courses**

The internal assessment of practical courses shall be conducted annually. There shall be one in-semester examination for practical courses. The examination shall be conducted annually. The in-semester assessment of practical courses shall have the following components.

<table>
<thead>
<tr>
<th>Component</th>
<th>Marks</th>
</tr>
</thead>
<tbody>
<tr>
<td>Attendance</td>
<td>5</td>
</tr>
<tr>
<td>Laboratory skills</td>
<td>5</td>
</tr>
<tr>
<td>Record</td>
<td>5</td>
</tr>
<tr>
<td>Test</td>
<td>10</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td><strong>25</strong></td>
</tr>
</tbody>
</table>

4.13 **Internal assessment of Project/Dissertation**

The project topics/supervisors shall be assigned well in advance, preferably in the beginning of third semester. Plagiarism shall be prevented in the dissertation. Internal valuation of project shall be performed by a committee consisting of Head of the Department, one senior faculty members and the concerned mentor.

<table>
<thead>
<tr>
<th>Component</th>
<th>Marks</th>
</tr>
</thead>
<tbody>
<tr>
<td>Content of work</td>
<td>10</td>
</tr>
<tr>
<td>Dissertation</td>
<td>5</td>
</tr>
<tr>
<td>Presentation and Viva</td>
<td>10</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td><strong>25</strong></td>
</tr>
</tbody>
</table>
4.14 **End-semester assessment**

The end-semester examination in theory and practical courses shall be conducted by the College.

4.15 The end-semester examinations for theory courses shall be conducted at the end of each semester. There shall be one end-semester examination of three (3) hours duration in each lecture based course.

4.16 The question paper should be strictly on the basis of model question paper set by Board of Studies.

4.17 A question paper consists of short answer type/annotation, short essay type questions/problems and long essay type questions.

<table>
<thead>
<tr>
<th>Division</th>
<th>Type</th>
<th>No. of Questions to be Answered</th>
<th>Mark for Each Question</th>
<th>Total Marks</th>
</tr>
</thead>
<tbody>
<tr>
<td>Part A</td>
<td>Short answer</td>
<td>10 out of 13</td>
<td>2</td>
<td>20</td>
</tr>
<tr>
<td>Part B</td>
<td>Short essay</td>
<td>5 out of 8</td>
<td>5</td>
<td>25</td>
</tr>
<tr>
<td>Part C</td>
<td>Essay</td>
<td>2 out of 4</td>
<td>15</td>
<td>30</td>
</tr>
<tr>
<td></td>
<td>Grand Total</td>
<td>17 out of 25</td>
<td>-</td>
<td>75</td>
</tr>
</tbody>
</table>

4.18 Photocopies of the answer scripts of the external examination shall be made available to the students for scrutiny as per the regulations in the examination manual.

4.19 Practical examination shall be conducted annually. The examination shall be conducted by one external examiner and one internal examiner. Practical examinations question papers will be set by the Chairman, Examination Boards.

4.20 All students shall give a seminar/report based on a research paper/review paper/journal article during their tenure of the programme and its report shall be submitted at the time of viva-voce. The research paper shall be selected in consultation with the Head of the Department/Academic Committee/Class Mentor/Project Supervisor.

4.21 Project evaluation shall be conducted at the end of the programme. Project evaluation shall be conducted by one external examiner and one internal examiner.

<table>
<thead>
<tr>
<th>Components of Project Evaluation</th>
<th>Marks</th>
</tr>
</thead>
<tbody>
<tr>
<td>Internal Evaluation</td>
<td>25</td>
</tr>
<tr>
<td>Dissertation (External)</td>
<td>50</td>
</tr>
<tr>
<td>Viva-Voce (External)</td>
<td>25</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td><strong>100</strong></td>
</tr>
</tbody>
</table>
4.22 Comprehensive viva-voce shall be conducted at the end of the programme. Viva-voce shall be conducted by one external examiner and one internal examiner. The viva-voce shall cover questions from all courses in the programme. There shall be no internal assessment for comprehensive viva-voce. The maximum marks for viva-voce is one hundred (100).

4.23 For all courses (theory and practical) an indirect grading system based on a ten (10) point scale according to the percentage of marks (ISA + ESA) is used to evaluate the performance of the student in that course. The percentage shall be rounded mathematically to the nearest whole number.

<table>
<thead>
<tr>
<th>Percentage of Marks</th>
<th>Grade</th>
<th>Performance</th>
<th>Grade Point</th>
</tr>
</thead>
<tbody>
<tr>
<td>90 and above</td>
<td>A+</td>
<td>Outstanding</td>
<td>10</td>
</tr>
<tr>
<td>80 - 89</td>
<td>A</td>
<td>Excellent</td>
<td>9</td>
</tr>
<tr>
<td>70 - 79</td>
<td>B</td>
<td>Very Good</td>
<td>8</td>
</tr>
<tr>
<td>60 - 69</td>
<td>C</td>
<td>Good</td>
<td>7</td>
</tr>
<tr>
<td>50 - 59</td>
<td>D</td>
<td>Satisfactory</td>
<td>6</td>
</tr>
<tr>
<td>40 - 49</td>
<td>E</td>
<td>Adequate</td>
<td>5</td>
</tr>
<tr>
<td>Below 40</td>
<td>F</td>
<td>Failure</td>
<td>-</td>
</tr>
</tbody>
</table>

4.24 **Credit Point**

Credit Point (CP) of a course is calculated using the formula

\[ CP = C \times GP \]

where \( C \) = Credit; \( GP \) = Grade Point

4.25 **Semester Credit Point Average**

Semester Credit Point Average (SCPA) is calculated using the formula

\[ SCPA = TCP/TC \]

where TCP = Total Credit Point of all the courses in the semester; TC = Total Credits in the semester

SCPA shall be rounded off to two decimal places.

4.26 **Cumulative Credit Point Average**

Cumulative Credit Point Average (CCPA) is calculated using the formula

\[ CCPA = TCP/TC \]

where TCP = Total Credit Point of all the courses in the whole programme; TC = Total Credit in the whole programme

CCPA shall be rounded off to two decimal places.
Grades for the different semesters; Semester Credit Point Average (SCPA) and overall programme; Cumulative Credit Point Average (CCPA) are given based on the corresponding Credit Point Average (CPA) as shown below:

<table>
<thead>
<tr>
<th>CPA</th>
<th>Grade</th>
<th>Performance</th>
</tr>
</thead>
<tbody>
<tr>
<td>9.00 and above</td>
<td>A+</td>
<td>Outstanding</td>
</tr>
<tr>
<td>8.00 - 8.99</td>
<td>A</td>
<td>Excellent</td>
</tr>
<tr>
<td>7.00 - 7.99</td>
<td>B</td>
<td>Very Good</td>
</tr>
<tr>
<td>6.00 - 6.99</td>
<td>C</td>
<td>Good</td>
</tr>
<tr>
<td>5.00 - 5.99</td>
<td>D</td>
<td>Satisfactory</td>
</tr>
<tr>
<td>4.00 - 4.99</td>
<td>E</td>
<td>Adequate</td>
</tr>
<tr>
<td>Below 4.00</td>
<td>F</td>
<td>Failure</td>
</tr>
</tbody>
</table>

4.27 A separate minimum of 30% marks each in ISA and ESA (for theory and practical) and aggregate minimum of 40% are required for a pass for a course. For a pass in a programme, a separate minimum of Grade E is required for all the individual courses.

5. SUPPLEMENTARY/IMPROVEMENT EXAMINATION
There will be supplementary examinations and chance for improvement. Only one chance will be given for improving the marks of a course.

6. ATTENDANCE
6.1 The minimum requirement of aggregate attendance during a semester for appearing the end semester examination shall be 75%. Condonation of shortage of attendance to a maximum of ten (10) days in a semester subject to a maximum of two times during the whole period of Postgraduate programme may be granted by the College.
6.2 If a student represents the College, University, State or Nation in Sports, NCC, NSS or Cultural or any other officially sponsored activities such as College union/University union activities, he/she shall be eligible to claim the attendance for the actual number of days participated subject to a maximum of ten (10) days in a semester based on the specific recommendations of the Faculty Mentor and Head of the Department.
6.3 A student who does not satisfy the requirements of attendance shall not be permitted to appear for the end-semester examinations.
6.4 Those students who are not eligible even with condonation of shortage of attendance shall repeat the course along with the next batch.

7. BOARD OF STUDIES AND COURSES
7.1 The Board of Studies in Chemistry shall design all the courses offered in the postgraduate programme in Chemistry. The Boards shall design and introduce new
courses, modify or re-design existing courses and replace any existing courses with new/modified courses to facilitate better exposure and training for the students.

7.2 The syllabus of a course shall include the title of the course, contact hours, the number of credits and reference materials.

7.3 Each course shall have an alpha numeric code which includes abbreviation of the course in two letters, the semester number, the code of the course and the serial number of the course.

7.4 Every Programme conducted under Credit Semester System shall be monitored by the Academic Council.

8. REGISTRATION

8.1 A student shall be permitted to register for the programme at the time of admission.

8.2 A student may be permitted to complete the Programme, on valid reasons, within a period of eight (8) continuous semesters from the date of commencement of the first semester of the programme.

8.3 Those students who possess the required minimum attendance and progress during an academic year/semester and could not register for the annual/semester examination in time are permitted to apply for Notional Registration to the examinations concerned enabling them to get promoted to the next semester.

9. ADMISSION

9.1 The admission to postgraduate programme in Chemistry shall be as per the rules and regulations of the College/University.

9.2 The eligibility criteria for admission shall be as announced by the College/University from time to time.

9.3 Separate rank lists shall be drawn up for seats under reservation quota as per the existing rules.

9.4 There shall be a uniform academic and examination calendar prepared by the College for the conduct of the programme.

10. ADMISSION REQUIREMENTS

10.1 Candidates for admission to the first semester of the postgraduate programme in Chemistry through SB-CSS-PG shall be required to have passed an appropriate degree examination of Mahatma Gandhi University or any University or authority, duly recognized by the Academic council of Mahatma Gandhi University as equivalent thereto.

10.2 Students admitted under this programme are governed by the Regulations in force.
11. PROMOTION
A student who registers for the end semester examination shall be promoted to the next semester.

12. MARK CUM GRADE CARD
12.1 The College under its seal shall issue to the students, a Mark cum Grade card on completion of each semester, which shall contain the following information.

   i) Name of the Student
   ii) Register Number
   iii) Photo of the Student
   iv) Degree
   v) Programme
   vi) Semester and Name of the Examination
   vii) Month and Year of Examination
   viii) Faculty
   ix) Course Code, Title and Credits of each course opted in the semester
   x) Marks for ISA, ESA, Total Marks (ISA + ESA), Maximum Marks, Letter Grade, Grade Point (GP), Credit Point (CP) and Institution Average in each course opted in the semester
   xi) Total Credits, Marks Awarded, Credit Point, SCPA and Letter Grade in the semester
   xii) Weighted Average Score
   xiii) Result

12.2 The final Mark cum Grade Card issued at the end of the final semester shall contain the details of all courses taken during the entire programme including those taken over and above the prescribed minimum credits for obtaining the degree. The final Mark cum Grade Card shall show the CCPA and the overall letter grade of a student for the entire programme.

13. AWARD OF DEGREE
The successful completion of all the courses with ‘E’ grade shall be the minimum requirement for the award of the degree.

14. MONITORING COMMITTEE
There shall be a Monitoring Committee constituted by the Principal to monitor the internal evaluation conducted by the College. The Course Teacher, Faculty Mentor, and the College Coordinator should keep all the records of the continuous evaluation, for at least a period of two years, for verification.
15. GRIEVANCE REDRESSAL COMMITTEE

15.1 In order to address the grievance of students relating to ISA, a two-level Grievance Redressal mechanism is envisaged.

15.2 A student can approach the upper level only if grievance is not addressed at the lower level.

15.3 Department level: The Principal shall form a Grievance Redressal Committee in each Department comprising of course teacher and one senior teacher as members and the Head of the Department as Chairman. The Committee shall address all grievances relating to the internal assessment grades of the students.

15.4 College level: There shall be a College level Grievance Redressal Committee comprising of Faculty Mentor, two senior teachers and two staff council members (one shall be an elected member) and the Principal as Chairman. The Committee shall address all grievances relating to the internal assessment grades of the students.

16. TRANSITORY PROVISION

Notwithstanding anything contained in these regulations, the Principal shall, for a period of three years from the date of coming into force of these regulations, have the power to provide by order that these regulations shall be applied to any programme with such modifications as may be necessary.
## MARK CUM GRADE CARD

**Name of the Candidate:**

**Register Number:**

**Degree:** Master of Science

**Programme:** Chemistry

**Name of the Examination:** First Semester SB-CSS-PG Examination, Month YYYY

**Faculty:** Science

<table>
<thead>
<tr>
<th>Course Code</th>
<th>Course Title</th>
<th>Credits (C)</th>
<th>ISA</th>
<th>ESA</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
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</table>

<table>
<thead>
<tr>
<th>Grade Awarded (G)</th>
<th>Credit Point (CP)</th>
<th>Institution Average Result</th>
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<tbody>
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</table>

**Total Weighted Average Score**

<table>
<thead>
<tr>
<th>Semester Result SCPA</th>
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</tbody>
</table>

***End of Statement***

Entered by:

Verified by:

**Controller of Examinations**

**Principal**
MARK CUM GRADE CARD

Name of the Candidate: 
Register Number: 
Degree: Master of Science
Programme: Chemistry
Name of the Examination: Fourth Semester SB-CSS-PG Examination, Month YYYY
Faculty: Science

<table>
<thead>
<tr>
<th>Course Code</th>
<th>Course Title</th>
<th>Credits (C)</th>
<th>ISA</th>
<th>ESA</th>
<th>Total</th>
<th>Grade Awarded (G)</th>
<th>Grade Point (GP)</th>
<th>Credit Point (CP)</th>
<th>Institution Average</th>
<th>Result</th>
</tr>
</thead>
<tbody>
<tr>
<td>Core Courses</td>
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<td>Elective Courses</td>
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<td>Project</td>
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<tr>
<td>Viva-Voce</td>
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***End of Statement***

Entered by: 
Verified by: 
Controller of Examinations: 
Principal:
Reverse side of the Mark cum Grade Card (COMMON FOR ALL SEMESTERS)

Description of the Evaluation Process - Grade and Grade Point

The evaluation of each course comprises of internal and external components in the ratio 1:3 for all Courses. Grades and Grade Points are given on a ten (10) point scale based on the percentage of Total Marks (ISA + ESA) as given in Table 1.

(Decimals are to be rounded mathematically to the nearest whole number)

<table>
<thead>
<tr>
<th>Percentage of Marks</th>
<th>Grade</th>
<th>Performance</th>
<th>Grade Point</th>
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<td>90 and above</td>
<td>A+</td>
<td>Outstanding</td>
<td>10</td>
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<tr>
<td>80 - 89</td>
<td>A</td>
<td>Excellent</td>
<td>9</td>
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<tr>
<td>70 - 79</td>
<td>B</td>
<td>Very Good</td>
<td>8</td>
</tr>
<tr>
<td>60 - 69</td>
<td>C</td>
<td>Good</td>
<td>7</td>
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<tr>
<td>50 - 59</td>
<td>D</td>
<td>Satisfactory</td>
<td>6</td>
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<tr>
<td>40 - 49</td>
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<td>Below 40</td>
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Table 1

Semester Credit Point Average (SCPA) and Cumulative Credit Point Average (CCPA)

Grades for the different Semesters and overall Programme are given based on the corresponding Credit Point Average (CPA), as shown in Table 2.

<table>
<thead>
<tr>
<th>CPA</th>
<th>Grade</th>
<th>Performance</th>
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<tr>
<td>9.00 and above</td>
<td>A+</td>
<td>Outstanding</td>
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<td>7.00 - 7.99</td>
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<td>6.00 - 6.99</td>
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<tr>
<td>5.00 - 5.99</td>
<td>D</td>
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<tr>
<td>Below 4.00</td>
<td>F</td>
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Table 2

Credit Point (CP) of a course is calculated using the formula

\[ CP = C \times GP \]

where \( C \) = Credit; \( GP \) = Grade Point

Credit Point Average (CPA) of a Semester/Programme is calculated using the formula

\[ CPA = \frac{TCP}{TC} \]

where \( TCP = \) Total Credit Point; \( TC = \) Total Credit

CPA shall be rounded off to two decimal places.

A separate minimum of 30% marks is required for a pass for both internal assessment and external assessment in each course.

An aggregate minimum of 40% marks is required for a pass in each course.
### PROGRAMME STRUCTURE

<table>
<thead>
<tr>
<th>Semester I</th>
<th>Course Code</th>
<th>Name of the Course</th>
<th>Hours /Week</th>
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| Grand Total |                |                    | 80          | 2300        |
ELECTIVE COURSES

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<td>AMCH4E03</td>
<td>Advanced Physical Chemistry</td>
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SEMESTER I

AMCH101: INORGANIC CHEMISTRY - I

Credits: 4

Contact Lecture Hours: 72

Unit 1: Metal Complexes: Structural Aspects and Bonding (18 hours)

1.1 Classification of complexes based on coordination numbers and possible geometries. Sigma and pi bonding ligands such as CO, NO, CN-, R3P, and Ar3P. Stability of complexes, thermodynamic aspects of complex formation-Irving-William order of stability, chelate effect.

1.2 Splitting of d orbitals in octahedral, tetrahedral, square planar, square pyramidal and trigonal bipyramidal fields, LFSE, Dq values, Jahn Teller (JT) effect, theoretical failure of crystal field theory, evidence of covalency in the metal-ligand bond, nephelauxetic effect, ligand field theory, molecular orbital theory-MO energy level diagrams for octahedral and tetrahedral complexes without and with π-bonding, experimental evidences for π-bonding.

Unit 2: Spectral and Magnetic Properties of Metal Complexes (18 hours)

2.1 Electronic Spectra of complexes-Term symbols of dn system, Racah parameters, splitting of terms in weak and strong octahedral and tetrahedral fields. Correlation diagrams for dₐ and d₁₀-ₐ ions in octahedral and tetrahedral fields (qualitative approach), d-d transition, selection rules for electronic transition-effect of spin-orbit coupling and vibronic coupling.

2.2 Interpretation of electronic spectra of complexes-Orgel diagrams, demerits of Orgel diagrams, Tanabe-Sugano diagrams, calculation of Dq, B and β (Nephelauxetic ratio) values, spectra of complexes with lower symmetries, charge transfer spectra, luminescence spectra.

2.3 Magnetic properties of complexes-paramagnetic and diamagnetic complexes, molar susceptibility, Gouy method for the determination of magnetic moment of complexes, spin only magnetic moment. Temperature dependence of magnetism-Curie’s law, Curie-Weiss law. Temperature Independent Paramagnetism (TIP), Spin state cross over, Antiferromagnetism-inter and intra molecular interaction. Anomalous magnetic moments.

2.4 Elucidating the structure of metal complexes (cobalt and nickel complexes) using electronic spectra, IR spectra and magnetic moments.
Unit 3: Kinetics and Mechanism of Reactions in Metal Complexes (18 hours)
3.1 Thermodynamic and kinetic stability, kinetics and mechanism of nucleophilic substitution reactions in square planar complexes, trans effect-theory and applications.
3.2 Kinetics and mechanism of octahedral substitution- water exchange, dissociative and associative mechanisms, base hydrolysis, racemization reactions, solvolytic reactions (acidic and basic).
3.3 Electron transfer reactions: outer sphere mechanism-Marcus theory, inner sphere mechanism-Taube mechanism.

Unit 4: Stereochemistry of Coordination Compounds (9 hours)
4.1 Geometrical and optical isomerism in octahedral complexes, resolution of optically active complexes, determination of absolute configuration of complexes by ORD and circular dichroism, stereoselectivity and conformation of chelate rings, asymmetric synthesis catalyzed by coordination compounds.

Unit 5: Coordination Chemistry of Lanthanides and Actinides (9 hours)
5.1 General characteristics of lanthanides-Electronic configuration, Term symbols for lanthanide ions, Oxidation state, Lanthanide contraction. Factors that mitigate against the formation of lanthanide complexes. Electronic spectra and magnetic properties of lanthanide complexes. Lanthanide complexes as shift reagents.
5.2 General characteristics of actinides-difference between 4f and 5f orbitals, comparative account of coordination chemistry of lanthanides and actinides with special reference to electronic spectra and magnetic properties.

Reference
Unit 1: Organic Reaction Mechanism  
1.1 Electronic Effects and their applications (detailed study): inductive effect, electromeric effect, resonance effect, hyperconjugation, steric effect steric acceleration and steric retardation. Allylic strain Bonding weaker than covalent bonds.
1.2 Reaction Intermediates- Generation, structure, stability and reactions of carbocations (classical and non classical), carbanions, radicals, carbenes (singlet and triplet- distinguishing reactions), nitrenes, benzynes. Hydrogen bonding and its effect of physical and chemical properties.
1.3 IUPAC Classification and Nomenclature of reaction mechanisms. Review of nucleophilic and electrophilic substitution at aliphatic carbon ($S_N^1$, $S_N^2$, $S_N^1'$, $S_N^2'$, $S_{Ni}$, $S_{E1}$, $S_{E2}$), effect of substrate, reagent, leaving group and solvent. Neighboring group participation-evidence, participation of phenonium, sigma and pi bonds. Elimination ($E_1$, $E_2$ & $E_{1CB}$). Elimination vs substitution.
1.4 Addition reactions (regioselectivity: Markovnikov’s addition-carcobcation mechanism, anti-Markovnikov’s addition-radical mechanism). Oxymercuration-demercuration, halolactonisation, hydroboration – oxidation. Addition to aromatic systems.
1.5 IUPAC nomenclature of organic molecules- simple, spiro compounds, bicyclo compounds, heterocyclic, benzenoid and non benzenoid compounds.

Unit 2: Aromaticity  
Consolidating different criteria for aromaticity- structural, electronic, energetic and magnetic criteria
2.2 Electrophilic Aromatic Substitution: Arenium ion mechanism, orientation and reactivity in monosubstituted benzene rings, ortho/para ratio, ipso attack.

Nucleophilic Aromatic substitution: $S_{N1}$, $S_{NAr}$, $SR_{N1}$ and Benzyne mechanisms, reactivity - effect of substrate structure, leaving group, and attacking nucleophile.

2.3 Organic reactions involving benzene diazonium salts- Meerwin reaction, Gomberg reaction, Pschorr reaction, coupling reactions: synthesis of azodyes, methyl red and methyl orange. Cloromethylation of aromatic systems- Gatterman’s formylation, Gateerman-Koch formylation, Hoesch acylation, Vilsmeier formylation, Reimer-Tiemann formylation, Kolbe-Schmidt carboxylation.

**Unit 3: Stereochemistry**

(18 hours)

3.1 Fischer, Newman, Sawhorse and Flying Wedge projections and their interconversions

3.2 Introduction to molecular symmetry and chirality: examples from common objects to molecules. Axis, plane, center, alternating axis of symmetry.

3.3 Center of chirality: molecules with C, N, S based chiral centers, absolute configuration, enantiomers, racemic modifications, R and S nomenclature using Cahn-Ingold-Prelog rules, molecules with a chiral center and Cn, molecules with more than one center of chirality, definition of diastereoisomers, constitutionally symmetrical and unsymmetrical chiral molecules, erythro, threo nomenclature.

3.4 Axial, planar and helical chirality with examples, stereochemistry and absolute configuration of allenes, biphenyls and binaphthyls, anise and cyclophane compounds, spiranes, exo-cyclic alkylidenecycloalkanes.

3.5 Topicity and prostereoisomerism, topicity of ligands and faces as well as their nomenclature. NMR distinction of enantiotopic/diastereotopic ligands.

3.6 Methods of resolution, optical purity and enantiomeric excess

3.7 Stereoisomerism: definition based on symmetry and energy criteria, configuration and conformational stereoisomers.

3.8 Geometrical isomerism: nomenclature, E-Z notation, methods of determination of geometrical isomers. Interconversion of geometrical isomers.

**Unit 4: Conformational Analysis**

(18 hours)

4.1 Conformational descriptors - factors affecting conformational stability of molecules. Conformational analysis of acyclic and cyclic systems: substituted ethanes, study of conformations of cyclohexane, mono, di and polysubstitutedcyclohexanes,cyclohexene,
cyclohexanone (2-alkyl and 3'-alkyl ketone effect), 2-halocyclohexanones, cyclopentane, cyclobutane, cycloheptane and cyclooctane, Conformation and anomeric effects in hexoses. Conformational structures of piperidine, N-Methylpiperidine, trope, trope, pseudotropine. Fused and bridged bicyclic systems, decalins, adamantane, hexamine, congressane, norborane etc.

4.2 Selection of substrate, Factors governing the reactivity of axial and equatorial substituents in cyclohexanes. Steric assisted and steric hindered reactions. Chemical consequence of conformational equilibrium - Curtin Hammett principle.

4.3 Effect of conformation on reactivity of cyclohexane derivatives in the following reactions (including mechanism): dehalogenation, dehydrohalogenation, semipinacolic deamination and pyrolytic elimination - (Saytzeff and Hofmann eliminations), nucleophilic substitutions, stereochemical addition to the carbonyl group of a rigid cyclohexanone, molecular rearrangements, formation and cleavage of epoxides, esterification and hydrolysis, reduction of cyclohexanones and oxidation of cyclohexanols.

Reference

Unit 1: Classical Thermodynamics

1.01 Entropy, dependence of entropy on variables of a system (S, T and V; S, T and P). Thermodynamic equations of state. Irreversible processes - Clausius inequality.
1.02 Free energy, Maxwell relations and significance, temperature dependence of free energy - Gibbs Helmholtz equation, applications of Gibbs Helmholtz equation.
1.03 Partial molar quantities, chemical potential and Gibbs-Duhem equations
1.04 Fugacity, relation between fugacity and pressure, determination of fugacity of a real gas, variation of fugacity with temperature and pressure. Activity, dependence of activity on temperature and pressure.
1.05 Thermodynamics of mixing, Gibbs-Duhem-Margules equation, Konowaloff’s rule, Henry’s law, excess thermodynamic functions-free energy, enthalpy, entropy and volume.
1.06 Chemical affinity and thermodynamic functions, effect of temperature and pressure on chemical equilibrium- vant Hoff reaction isochore and isotherm. Clausius and Clapeyron equation and its application for the determination of colligative properties (depression in freezing point, elevation in boiling point and relative lowering of vapour pressure). Determination of molecular weight of non – volatile solutes from colligative properties. Relationship between relative lowering of vapour pressure and osmotic pressure. Van’t Hoff equation for dilute solutions and its application.
1.07 Third law of thermodynamics, Nernst heat theorem, determination of absolute entropies using third law, entropy changes in chemical reactions.
1.08 Three component systems-graphical representation. Solid-liquid equilibria ternary solutions with common ions, hydrate formation, compound formation. Liquid-liquid equilibria-one pair of partially miscible liquids, two pairs of partially miscible liquids, three pairs of partially miscible liquids.
1.09 Thermodynamics of irreversible processes with simple examples. Uncompensated heat and its physical significance. Entropy production- rate of entropy production, entropy production in chemical reactions, the phenomenological relations. The principle of microscopic reversibility, the Onsager reciprocal relations (no derivation).Thermal osmosis. Thermoelectric phenomena.
1.10 Bioenergetics: coupled reactions, ATP and its role in bioenergetics, high energy bond, free energy and entropy change in ATP hydrolysis, thermodynamic aspects of metabolism and respiration, glycolysis, biological redox reactions.

**Unit 2: Statistical Thermodynamics** (27 hours)

2.1 Permutation, probability, apriori and thermodynamic probability, Sterlings approximation, macrostates and microstates, Boltzmann distribution law, partition function and its physical significance, phase space, different ensembles, canonical partition function, distinguishable and indistinguishable molecules, partition function and thermodynamic functions, separation of partition function- translational, rotational, vibrational and electronic partition functions. Thermalde-Broglie wavelength. Equilibrium constant in terms of partition functions.

2.2 Calculation of thermodynamic functions. Sakur-Tetrode equation, statistical formulation of third law of thermodynamics, thermodynamic probability and entropy, residual entropy, heat capacity of gases - classical and quantum theories, heat capacity of hydrogen.

2.3 Need for quantum statistics, Bose-Einstein statistics: Bose-Einstein distribution, example of particles, Bose-Einstein condensation (basic idea), liquid helium, supercooled liquids. Fermi- Dirac distribution: examples of particles, application in electron gas, thermionic emission. Comparison of three statistics.

2.4 Heat capacity of solids- the vibrational properties of solids, Einstein’s theory and its limitations, Debye theory and its limitations.

**Reference**

AMCH104: THEORETICAL CHEMISTRY - I

Credits: 4
Contact Lecture Hours: 72

Unit 1: Basics of Quantum Mechanics (12 hours)
1.1 Wave Function, Born interpretation of the wave function, Acceptable Wave Functions, Normalization, Orthogonal Functions, Orthonormality, Operators, Construction of Operators, Hermitian Operators and their properties, Eigen functions and Eigen values; State function postulate, operator postulate, expectation value and other postulates; Time-dependent Schrödinger Wave Equation, Time-independent Schrödinger Wave Equation from Classical Wave equation.

1.2 Atomic Orbitals: Hydrogen like, Slater and Gaussian type AOs, Plots and general features; Slater Determinants, examples and significance; Pauli’s Exclusion Principle.
Quantum Mechanical Tunneling: Concept, transmission coefficient, examples; Spin-Orbitals: Concept, Spin and Orbital functions, Construction of spin orbitals with simple examples; Spin-angular momentum, its orientations; Stern-Gerlach Experiment and its significance; Hellmann-Feynmann theorem, Applications.

Unit 2: Applications of Quantum Mechanics to Simple Chemical Systems (24 hours)
2.1 Quantum mechanics of a free particle in motion; Particle on a ring: Circular Harmonics, Normalized wave functions, quantization of energy.

2.2 Particle in one dimensional box with infinite potential walls, normalized wave functions, calculation of energy; Particle in a 3D box: Calculation of Energy, Degeneracy; Quantum Mechanics of Harmonic Oscillator: Hermite Polynomials (elementary ideas only), Normalized wave functions, comparison between classical and harmonic oscillators; Non-planar Rigid Rotor: Rigid rotor approximation, Schrödinger Wave Equation for Rigid Rotor, Mathematical treatment, Phi and Theta equations, solutions; Concept of Spherical Harmonics: Examples, Polar diagrams, S- and P- functions and their mathematical forms.

2.3 Quantum Mechanics of Hydrogen like Systems: Hydrogen atom, Hamiltonian in spherical polar coordinates, Schrödinger Wave Equation, Separation of variables, Radial and
Angular equations and their solutions (derivation of l and m only); Radial and angular functions for 1s, 2s and 2p orbitals. Symmetric and antisymmetric wave functions. The postulate of spin by Uhlenbeck and Goudsmith, discovery of spin-Stern Gerlach experiment. Spin orbitals-construction of spin orbitals from orbitals and spin function.

**Unit 3: Symmetry and Groups**

Symmetry elements, symmetry operations, point groups, classes, abelian and cyclic groups, group multiplication tables-classes in a group and similarity transformation. Symmetry in crystals-32 crystallographic point groups (no derivation), Hermann-Mauguin symbols. Space groups: Screw axis and Glide plane, determination of space group symbols of triclinic and monoclinic systems.

**Unit 4: Theory of Molecular Symmetry**

Matrix representation of symmetry operations, construction of representation using vectors and atomic orbitals as basis, representation generated by Cartesian coordinates positioned on the atoms of a molecule (C_{2v}, C_{3v} and D_{3h} as examples). Reducible and irreducible representations-construction of irreducible representation by standard reduction formula. Statement of Great Orthogonality Theorem (GOT).Properties of irreducible representations. Construction of irreducible representation using GOT-construction of character tables for C_{2v}, C_{2h}, C_{3}, C_{3v} and C_{4v}. Direct product of representations and its application. Molecular dissymmetry and optical activity.

**Unit 5: Application of Group Theory in Spectroscopy**

Applications in vibrational spectra: transition moment integral, vanishing of integrals, symmetry aspects of molecular vibrations, vibrations of polyatomic molecules-selection rules for vibrational absorption. Normal mode analysis of H_{2}O, Trans N_{2}F_{2} and NH_{3} using Cartesian coordinates and internal coordinate methods. Complementary character of IR and Raman spectra-determination of the number of active IR and Raman lines. Application in electronic spectra: selection rules for electronic transition, electronic transitions due to the carbonyl chromophore in formaldehyde.

**Reference**

Unit 1: Organometallic Compounds-Synthesis, Structure and Bonding (18 hours)
1.1 Organometallic compounds with linear pi donor ligands—olefins, acetylenes, dienes and allyl complexes—synthesis, structure and bonding.
1.2 Complexes with cyclic pi donors—metallocenes and cyclic arene complexes—structure and bonding. Hapto nomenclature. Carbene and carbyne complexes.
1.3 Preparation, properties, structure and bonding of simple mono and binuclear metalcarbonyls, metal nitrosyls, metal cyanides and dinitrogen complexes. Polynuclearmetal carbonyls with and without bridging. Carbonyl clusters-LNCCS and HNCCS, Isoelectronic and isolobal analogy, Wade-Mingos rules, cluster valence electrons.

Unit 2: Reactions of Organometallic Compounds (9 hours)
2.1 Substitution reactions—nucleophilic ligand substitution, nucleophilic and electrophilic attack on coordinated ligands.
2.2 Addition and elimination reactions—1,2 additions to double bonds, carbonylation and decarbonylation, oxidative addition and reductive elimination, insertion(migration) and elimination reactions.
2.3 Rearrangement reactions, redistribution reactions, fluxional isomerism.

Unit 3: Catalysis by Organometallic Compounds (9 hours)
3.1 Homogeneous and heterogeneous organometallic catalysis—alkene hydrogenation using Wilkinson catalyst, Tolman catalytic loops.
3.2 Reactions of carbon monoxide and hydrogen—the water gas shift reaction, the Fischer-Tropsch reaction (synthesis of gasoline), hydroformylation of olefins using cobalt or rhodium catalyst. Polymerization by organometallic initiators and templates for chain propagation—Ziegler Natta catalysts.
3.3 Carbonylation reactions—Monsanto acetic acid process, carbonylation of butadiene using Co₂(CO)₈ catalyst in adipic ester synthesis. Olefin methathesis-synthesis gas based
reactions, photodehydrogenation catalyst (“platinum pop”). Palladium catalysed oxidation of ethylene-the Wacker process.

**Unit 4: Biocoordination Chemistry**

<table>
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<th>18 hours</th>
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<tr>
<td><strong>4.1</strong> Metals in Biological Systems: Bulk, trace and ultra trace metals for living systems, their biological roles, response of organisms to varying concentrations of these metals.</td>
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<tr>
<td><strong>4.2</strong> Chemical Toxicology: Biochemical effects of the metals: Arsenic, Cadmium, Lead and Mercury.</td>
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<td><strong>4.3</strong> Chemistry of Photosynthesis: Light reactions: Reaction center, photosystem, Z-Scheme, Photosystem I and II, structure and function of Mn cluster.</td>
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<td><strong>4.4</strong> Metal Management in Living Systems: Iron Storage: Ferritin, Haemosiderin; Iron Transport: Transferrins, Siderophores and their iron transfer mechanisms</td>
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<tr>
<td><strong>4.5</strong> Electron Transfer in Biological Systems: Blue copper proteins; Fe-S proteins: Rubredoxins and Ferredoxins; Cytochromes: Classification, structure and functions of cytochrome c, cytochrome c-oxidase and cytochrome b6f complex.</td>
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<td><strong>4.6</strong> Nitrogen Fixation: Diazotrophs, Symbiosis, Nitrogenases and their components, Chemistry of biological nitrogen fixation,</td>
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<tr>
<td><strong>4.7</strong> Metalloenzymes: Structure and functions of Superoxide dismutases, Carbonic anhydrase II, Carboxypeptidase A, Peroxidases, Catalases, Oxidases, and Oxygenases. Cytochrome P450, its mode of action in drug metabolism, tyrosinases, Ribonucleotidereductase, Coenzyme forms of vitamin B12: structures and functions.</td>
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<tr>
<td><strong>4.8</strong> Metals in Medicine: Metals as radiation sources: radio nuclides, common examples; Cis-platin: its mode of action in cancer treatment; Contrasting Agents in MRI, Gadolinium based contrasting agents, simple examples using cyclen like macrocyclic ligands, their mode of action; Application of therapeutic chelating agents: Basic principles of chelation therapy with examples; Chrysotherapy: Antiarthritic agents containing gold.</td>
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**Unit 5: Nuclear Chemistry**

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<tr>
<td><strong>5.1</strong> Radioactive equilibrium: Transient and secular equilibria. Q value, reaction cross sections, threshold energy. Nuclear structure, mass and charge. Nuclear models – shell, liquid</td>
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drop, Fermi gas, collective and optical models. Nuclear moments, nuclear forces, binding energy. Semiempirical mass equation. Stability rules, Magic numbers


5.3 Synthesis of transuranic elements such as Neptunium, Plutonium, Curium, Berkelium, Einsteinium, Mendelevium, Nobelium, Lawrencium and elements with atomic numbers 104 to 109.

5.4 Analytical applications of radioisotopes-radiometric titrations, kinetics of exchange reactions, measurement of physical constants including diffusion constants, Radioanalysis, Neutron Activation Analysis, Prompt Gama Neutron Activation Analysis and Neutron Absorptiometry.

5.5 Applications of radio isotopes in industry, medicine, autoradiography, radiopharmacology, radiation safety precaution, nuclear waste disposal. Radiation chemistry of water and aqueous solutions.

5.6 Measurement of radiation doses. Relevance of radiation chemistry in biology, organic compounds and radiation polymerization.

Reference

10. UN Gosh Nuclear Chemistry, S Chand & Sons, 2005
AMCH206: ORGANIC CHEMISTRY - II

Unit 1: Physical Organic Chemistry (18 hours)


1.2 Structural effects and reactivity: Linear free energy relationship (LFER) in determination of organic reaction mechanism, The Hammett equation, substituent constants, theories of substituent effects, interpretation of σ-values, reaction constants ρ. The Taft model, Solvent effects.

1.3 Specific and general catalysis, Acid-base catalysis: General methods of investigating mechanisms. Catalysis by acids and bases and nucleophiles with examples from acetal, cyanohydrin and ester formation and hydrolysis reactions-AAC2, AAC1, AAL1, BAC2and BAL1 mechanisms. Phase transfer catalysis and applications, Solvent effect. Bulk and specific solvent effects. Kinetic isotope effects with examples. Effect of structure and solvent on acidity and basicity

Reference

5. Modern physical chemistry, Eric V Anslyn, Dennis A. Dougherty, University science books,2006

Unit 2: Concerted Reactions (18 hours)

2.1 Pericyclic Reactions: Classification, electrocyclic, sigmatropic, cycloaddition, chelotropic and ene reactions, Woodward Hoffmann rules, Frontier Orbital and Orbital
symmetry correlation approaches, examples highlighting pericyclic reactions in organic synthesis such as Claisen, Cope, Wittig, Mislow-Evans and Sommelet-Hauser rearrangements, Diels-Alder and Ene reactions (with stereochemical aspects), introductory dipolar cycloaddition.

2.2 Unimolecular pyrolytic elimination reactions: Cheletropic elimination, Decomposition of cyclic azo compounds, b-eliminations involving cyclic transition states such as sulfoxides, selenoxides, N-oxides, acetates, xanthates eliminations. Problems based on the above reactions. [1, 2] Sigmatropic rearrangements to cationic centers; [2, 3] Sulfur Ylide Rearrangement Using a Chiral Auxiliary; Meisenheimer Rearrangement; [2, 3] Sigmatropic Rearrangements: Ring Expansion & Contraction; Stereo selectivity in cope rearrangements; Walk rearrangements Chirality transfer in Claisen rearrangements, Molecules with "fluxional" structures (bullvalene, homotropilidene etc.) Periselectivity and exo selectivity in Cycloadditions

Reference
2. S. Sankararaman, Pericyclic Reactions-A Text Book, Wiley VCH, 2005

Unit 3: Enolates and enamines- (18 hours)

3.2 Malonic acid esters- alkylation, decarboxylation, conjugate addition, Knoevenagel & Doebner condensation. Beta keto esters- Claisen condensation, Deickman & Stobbe condensation, Acyloin condensation, Tandem Dieckman condensation for the synthesis of 1,2, 1,3 and 1,4 –dienones. Synthesis of acetoacetic esters. Alkylation and decarboxylation of beta keto esters. Perkin reaction, Darzen reaction, Thorpe reaction. Mitsunobu reaction,

3.4 Cyclic ketone alkylation, imine and hydrazone anions- Claisen- Schmidt, Condensation reactions of enols and enamines- Mannich reaction- amino methylation, enone synthesis. Michael addition-acid and base catalysed and intra molecular, Robinson’s annulations- regioselectivity.

Reference

Unit 4: Some organic named reactions (18 hours)
Mechanisms and applications (evidences not expected)

Reference
1. ROC Norman and JM Coxon, Principles of Organic Synthesis. CRC Press
5. Jie Jack Li Name Reactions, Springer India, New Delhi, 4th Ed. (2011)
Unit 1: Foundations of Spectroscopic Techniques

1.1 Origin of spectra: origin of different spectra and the regions of the electromagnetic spectrum, intensity of absorption, influencing factors, signal to noise ratio, natural line width, contributing factors, Doppler broadening, Born Oppenheimer approximation

1.2 Microwave spectroscopy: principal moments of inertia and classification (linear, symmetric tops, spherical tops and asymmetric tops), selection rules, intensity of rotational lines, relative population of energy levels, derivation of Jmax, effect of isotopic substitution, calculation of intermolecular distance, spectrum of non rigid rotors, rotational spectra of polyatomic molecules, linear and symmetric top molecules, Stark effect and its application, basic instrumentation, chemical analysis by microwave spectroscopy.

1.3 Infrared spectroscopy: Morse potential energy diagram, fundamentals, overtones and hot bands, determination of force constant, diatomic vibrating rotator, vibrational spectra of polyatomic molecules, normal modes of vibrations, combination and difference bands, Fermi resonance, finger print region and group vibrations, effect of H-bonding on group frequency, introduction to FT spectroscopy, FTIR, ATR, Sampling.

1.4 Raman spectroscopy: scattering of light, polarizability and classical theory of Raman spectrum, rotational and vibrational Raman spectrum, complementarities of Raman and IR spectra, mutual exclusion principle, polarized and depolarized Raman lines, resonance Raman scattering and resonance fluorescence.

1.5 Electronic spectroscopy: term symbols of diatomic molecules, electronic spectra of diatomic molecules, selection rules, vibrational coarse structure and rotational fine structure of electronic spectrum, Franck-Condon principle, predissociation, calculation of heat of dissociation, Birge and Sponer method, different types of lasers-solid state lasers, continuous wave lasers, gas lasers and chemical laser, frequency doubling, applications of lasers

Unit 2: Resonance Techniques

2.1 NMR spectroscopy: interaction between nuclear spin and applied magnetic field, nuclear energy levels, population of energy levels, Larmor precession, chemical shift, representation, examples of AB, AX and AMX types, exchange phenomenon, factors influencing coupling, Karplus relationship.
2.2 FTNMR, relaxation methods and their determination, second order effects on spectra, spin systems (AB, AX, AMX, ABC), simplification of second order spectra, chemical shift reagents, high field NMR, double resonance, NOE effect, two dimensional NMR, COSY and HETCOR, $^{13}$C NMR, $^{13}$C chemical shift and structure correlation, introduction to solid state NMR, magic angle spinning.

2.3 EPR spectroscopy: electron spin in molecules, interaction with magnetic field, g factor, factors affecting g values, fine structure and hyperfine structure, Kramers’ degeneracy, McConnell equation; Applications.

2.4 An elementary study of NQR spectroscopy. Its effect on NMR spectrum. Applications.

2.5 Mossbauer spectroscopy: principle, Doppler effect, recording of spectrum, chemical shift, factors determining chemical shift, application to metal complexes, MB spectra of Fe(II) and Fe(III) cyanides.

**Unit 3: Crystallography**

(18 hours)

3.1 Miller indices, point groups (derivation not expected), translational symmetry, glide planes and screw axes, space groups, simple cases like triclinic and monoclinic systems, interplanar spacing and method of determining lattice types, reciprocal lattices, methods of characterizing crystal structure, rotating crystal method, powder X-ray diffraction method, determination of structure of sodium chloride by powder method, comparison of the structures of NaCl and KCl, brief outline of single crystal X-ray diffraction and crystal growth techniques.

3.2 Structure factor: atomic scattering factor, coordinate expression for structure factor, structure by Fourier synthesis.

3.3 Liquid crystals: mesomorphic state, types, examples and application of liquid crystals. Theories of liquid crystals. Photoconductivity of liquid crystals

**Reference**

AMCH208: THEORETICAL CHEMISTRY - II

Credits: 3
Contact Lecture Hours: 54

Unit 1: Approximation methods (18 hours)
1.1 Independent Particle Model: Example of Helium atom, Electron correlation problem, Calculation of ground state energy, Comparison with experimental value.
1.2 Variation Method: Variation theorem and proof, Rayleigh Ratio, Rayleigh-Ritz Method, Illustration with simple trial functions [x (a-x) for particle in 1D box, exp (-ar) for Hydrogen atom], Application of Variation theorem to Helium atom, Calculation of ground state energy, Comparison with experimental value.
1.3 Perturbation Method: General Concept, Time-independent perturbation method, non-degenerate case, first-order correction to energy and wave functions with derivations; Examples: Helium atom, Particle in a 1 D box with slanted bottom, anharmonic oscillator
1.4 Self-Consistent Field Methods: General Concepts and Algorithm for HSCF method, Concept of Basis functions, Roothan-Hall equations, Hartree-Fock Self consistent field method: Algorithm.

Unit 2: Chemical Bonding (18 hours)
2.1 Valence Bond Theory: Basic principles, Hydrogen molecule, its singlet and triplet state functions. Molecular Orbital Theory: Representation of MOs, separated atom and united atom approaches, Correlation diagrams, non-crossing rules, MOT of Hydrogen Molecule and its ion, Molecular Term symbols. Comparison of VB and MO theories. Molecular Orbital (MO) theory, MO theory of H_2^+ ion, MO theory of H_2 molecule, MO treatment of homonuclear diatomic molecules Li_2, Be_2, N_2, O_2 and F_2 and hetero nuclear diatomic molecules LiH, CO, NO and HF. Bond order. Correlation diagrams, non-crossing rule. Spectroscopic term symbols for diatomic molecules.
2.2 Hybridization: Quantum Mechanics of sp, sp^2 and sp^3 hybridizations. Hückel Molecular Orbital Method: Basics, Application to Ethylene, Butadiene, Benzene, Allyl and Cyclopropenyl Systems; Charge on an atom: Calculation of total electron density, Charge density, pi-bond order and free valence index.

Unit 3 Gaseous State (9 hours)
3.1 Derivation of Maxwell’s law of distribution of velocities, graphical representation, experimental verification of the law, most probable velocity, derivation of average, RMS and
most probable velocities, collision diameter, collision frequency in a single gas and in a mixture of two gases, mean free path, frequency of collision, effusion, the rate of effusion, time dependence of pressure of an effusing gas, the law of corresponding states, transport properties of gases.

**Unit 4: Applications of Group Theory in Chemical Bonding**

(9 hours)

Application in quantum mechanics, transition moment integral, vanishing of integrals. Applications in chemical bonding, construction of hybrid orbitals with BF$_3$, CH$_4$, PCl$_5$, XeF$_4$ as examples. Transformation properties of atomic orbitals. Symmetry adapted linear combinations (SALC) of C$_{2v}$, C$_{2h}$, C$_3$, C$_{3v}$ and D$_{3h}$. Jahn-Teller effect. Woodward Hoffmann rules-correlation diagram.

**Reference**

2. P.W. Atkins, R.S. Friedman, Molecular Quantum Mechanics, 4$^{th}$ Edn., Oxford University Press, 2005.
Ltd, 2013 Edn.
SEMMESTERS I AND II

PRACTICAL

AMCH2P01: INORGANIC CHEMISTRY PRACTICAL - I

Credits: 3  Contact Lab Hours: 54+54=108

PART I
Separation and identification of four metal ions including two less familiar metal ions such as Tl, W, Se, Mo, Ce, Th, Ti, Zr, V, U and Li. Anions which need elimination not to be given. A minimum of 5 mixtures containing 5 different less common ions shall be analysed by a student.

PART II
Colorimetric estimation of Fe, Cu, Ni, Mn, Cr, NH₄⁺, nitrate and phosphate ions.

PART III
Preparation and characterization complexes using IR, NMR and electronicspectra.
(i) Tris(thiourea)copper(I) complex
(ii) Potassium tris(oxalato) aluminate (III).
(iii) Hexammine cobalt (III) chloride.
(iv) Tetrammine copper (II) sulphate.
(v) Schiff base complexes of various divalent metal ions.

Reference
AMCH2P02: ORGANIC CHEMISTRY PRACTICAL - I

Credits: 3
Contact Lab Hours: 54+54=108

1. Separation of binary and ternary mixtures using chemical and physical methods
   Ether, bicarbonate, NaOH, HCl and bisulphite separation.
   (Minimum: binary - 2, ternary-4)

2. One stage and two stage synthesis
   a. Synthesis of the following (single stage) (some examples)
      1. Methyl orange from sulphanilic acid
      2. Azobenzene from beta naphthol
      3. Benzyl alcohol and benzoic acid by Cannizaro’s reaction
      4. Ethyl acetoacetate by Claisen condensation
      5. O and p hydroxyl acetophenone by Fries reaction
      6. 1-chloro 2,4-dinitro benzene from chlorobenzene
      7. 3,5-dinitrobenzoic acid from benzoic acid
      8. Cinnamic acid by Perkins reaction
      9. Oxalic acid from cane sugar
     10. Dimethyl phthalate
   
   b. Two stage synthesis (some examples)
      1. Aniline- diazoaminobenzene- p-aminoazo benzene
      2. Benzophenone- oxime- benzanilide (Beckman rearrangement)
      3. Phthalic anhydride- phthalimide-anthranilic acid (Hofmann rearrangement)
      4. Acetanilide- parabromoacetaldehyde- para bromo aniline
      5. Acetanilide- paranitroacetaldeyde- para nitro aniline
      6. Nitrobenzene- metadinotrobenzene-meta nitroaniline
      7. Chlorobenzene- 1-chloro 2,4-dinitrobenzene- 2,4-dinitrophenylhydrazine
      8. Phthalic anhydride- fluorescein- eosin
      9. P-toludine- p-cholorotoluene- p-chlorobenzoic acid
     10. Dimethyl aniline- p-nitrosodimethylaniline- methylene blue
(Single stage minimum – 5; double stage minimum – 5)
(Recrystallized samples/crude samples of the final product shall be exhibited during examination)

3. Chemical Structure drawing using software
   Use of structure drawing software to draw the reaction scheme including mechanisms of reactions.

Reference
Graphs may be drawn manually or using spreadsheets.

I. Adsorption
1. Verification of Freundlich and Langmuir adsorption isotherm: charcoal-acetic acid or charcoal-oxalic acid system.
2. Determination of the concentration of the given acid using the isotherms.

II. Phase diagrams
1. Construction of phase diagrams of simple eutectics.
   c. Construction of phase diagram of compounds with congruent melting point: diphenyl amine-benzophenone system.
2. Effect of (KCl/succinic acid) on miscibility temperature.
   d. Construction of phase diagrams of three component systems with one pair of partially miscible liquids.

III. Distribution law
1. Distribution coefficient of iodine between an organic solvent and water.
2. Distribution coefficient of benzoic acid between benzene and water.
3. Determination of the equilibrium constant of the reaction KI + I₂ ↔ KI₃

IV. Surface tension
1. Determination of the surface tension of a liquid by
   a) Capillary rise method
   b) Drop number method
   c) Drop weight method
2. Determination of parachor values.
3. Determination of the composition of two liquids by surface tension measurements

V Viscosity
1. Determination of viscosity of pure liquids.
2. Verification of Kendall’s equation.
SEMESTER III

AMCH309: INORGANIC CHEMISTRY - III

Credits: 4 Contact Lecture Hours: 72

Unit 1: Solid State Chemistry (18 hours)

1.1 Structure of solids: Imperfections in solids-point defects, line defects and plane defects. Structure of compounds of AX (Zinc blende, Wurtzite), AX₂ (Rutile, fluorite, antifluorite), AmX₂ (Nickel Arsenide), ABX₃ (Perosvskite, Ilmenite). Spinels, Inverse spinel structures.
1.2 Solid state reactions-diffusion coefficient, mechanisms, vacancy diffusion, thermal decomposition of solid-Type I reactions, Type II reactions.

Unit 2: Electrical, Magnetic and Optical Properties (18 hours)

2.2 Magnetic properties of transition metal oxides, garnets, spinels, ilmenites and perovskites, magnetoplumbites.
2.3 Optical properties-photoconductivity, photovoltaic effects, luminescence. Applications of optical properties.
2.4 Super conductivity-Type I and Type II superconductors, Frolich diagram, Cooper pairs, theory of low temperature super conductors, junctions using superconductors, BCS theory of superconductivity (derivation not required). Superconducting cuprates - YBaCu oxide system, Meisner effect, conventional superconductors, organic superconductors, fullerenes, carbon nanotubes, high temperature superconductors.
Unit 3: Inorganic Chains and Rings  
(18 hours)


3.2 Rings-topological approach to boron hydrides, Styx numbers. Structure and bonding in borazines, ring silicates and silicones, phosphorous-nitrogen compounds, phosphazenes. Heterocyclic inorganic ring systems-structure and bonding in phosphorous-sulphur and sulphur-nitrogen compounds. Homocyclic inorganic ring systems-structure and bonding in sulphur, selenium and phosphorous compounds.

Unit 4: Inorganic Cages and Metal Clusters  
(9 hours)

4.1 Cages: synthesis, structure and bonding of cage like structures of phosphorour. Boron cage compounds-Wade Mingos Lauher rules, MNO rule, boranes, carboranes, metallacarboranes.

4.2 Metal clusters: dinuclear compounds of Re, Cu and Cr, metal-metal multiple bonding in (Re$_2$X$_8$)$_2^-$, trinuclear clusters, tetranuclear clusters, hexanuclear clusters. Polyatomic zintl anion and cations. Infinite metal chains.

Unit 5: Chemistry of Materials  
(9 hours)

5.1 Glasses, ceramics, composites, nanomaterials-preparative procedures. Sol-gel synthesis, glassy state-glass formers and glass modifiers, ceramics-structure, mechanical properties, clay products, refractories- characterizations, properties and applications.

Reference

Unit 1: Oxidation and Reduction methods (18 hours)
1.1 Oxidation: Metal based and non-metal based oxidations of (a) alcohols to carbonyls (Chromium, Manganese, aluminium, silver, ruthenium. DMSO, hypervalent iodine and TEMPO based reagents, Jones, Collins-Ratcliff reagents, PCC, PDC, Swern oxidation) Dess-Martin Periodinane oxidation, tetrapropylammonium perpethenate-TPAP, barium manganate. (b) phenols (Fremy’s salt, silver carbonate on Celite (Fetizon’s reagent)) (c) alkenes to epoxides (peroxides/per acids based), Sharpless asymmetric epoxidation, Jacobsen epoxidation, Shi epoxidation. (d) alkenes to diols (Manganese, Osmium based), Sharpless asymmetric dihydroxylation, Prevost reaction and Woodward modification, (e) alkenes to carbonyls with bond cleavage (Manganese, Osmium, Ruthenium and lead based, ozonolysis) (f) alkenes to alcohols/carbonyls without bond cleavage (hydroboration-oxidation, Wacker oxidation, selenium, chromium based allylic oxidation) (g) ketones to ester/lactones (Baeyer-Villiger), Babler oxidation.

1.2 Reduction: (a) Catalytic hydrogenation (Heterogeneous: Palladium/Platinum/Rhodium/Nickel etc; Homogeneous: Wilkinson). Noyori asymmetric hydrogenation (b) Metal based reductions using Li/Na/Ca in liquid ammonia, Sodium, Magnesium, Zinc, Titanium and Samarium (Birch, Pinacol formation, McMurry, Acyloin formation, dehalgenation and deoxygenations) (c) Hydride transfer reagents from Group III and Group IV in reductions. (i) NaBH₄ triacetoxyborohydride, L-selectride, K-selectride, Luche reduction; LiAlH₄, DIBAL-H, and Red-Al, Trialkylsilanes and Trialkylstannane, Meerwein-Pondorff-Verley reduction) (ii) Stereo/enantioselectiviey reductions (Chiral Boranes, Corey-Bakshi-Shibata).

Unit 2: Protecting Functional Groups and Reagents (9 hours)
Protection and deprotection of NH (N-benzylamines, amides, carbamates, benzyloxy carbonyl, Boc, Fmoc), OH (alkyl ethers, benzylic ethers, trityl ethers, silyl ethers, acetics, esters), 1,2 and 1,3 diols as acetals, carbonyl groups, carboxyl group (alkyl, aryl, silyl esters, oxazolines), double bond and triple bond.
Lithium diisopropylamide (LDA), Dicyclohexyl carbodiimide (DDC), 1,3-Dithiane (Umpolung reagent), DDQ, Trimethylsilyl iodide, Phase transfer catalysts: Quaternary ammonium and phosphonium salts, Crown ethers, Gilman Reagent

**Unit 3: Organic Photochemistry (9 hours)**

Photochemistry of \((\pi, \pi^*)\) transitions: Excited states of alkenes, cis-trans isomerisation, electrocyclisation and sigmatropic rearrangements, di-\(\pi\) methane rearrangement. Intermolecular reactions, photocycloadditions, photodimerisation of simple and conjugated olefins, addition of olefins to \(\alpha, \beta\)-unsaturated carbonyl compounds. Photochemistry of aromatic compounds: Ring isomerization and cyclization reactions.

Photochemistry of \((n-\pi^*)\) transitions: Excited states of carbonyl compounds, homolytic cleavage of \(\alpha\)-bond, Norrish type I reactions in acyclic and cyclic ketones and strained cycloalkanедiones. Photo Fries rearrangements


**Reference**


**Unit 4: Organometallic Reagents in Organic Synthesis (18 hours)**

4.1 Use of organolithium agents: Preparation, reactivity, lithium halogen exchange, transmetalation, metalation, chemoselectivity, benzilic and allylic metallation, metallation of alpha–heteroatom substituted alkenes and 1-alkynes, conjugate addition. Organo magnesium reagents: Grignard Reagents- preparation and reactions.

4.2 Organotitanium reagents: Tebbe olefination, Zeigler's reagent. Organocerium reagents, Organocopper reagents: Preparation and reaction of organic cuprates. Conjugate addition, Tandem 1,4- addition by enolate trapping, O trapping, C trapping, preparations of enones.

Organo cobalt reagents- Pauson-Khand reaction

Organochromium reagents: Nosaki-Hiyama Reaction, Nozaki Takai Hiyama Kishi Coupling.
Organo zinc reagents: Preparation and reactions- Reactions of functionally substituted RZnI.
Organo boron reagents: carbonylation, synthesis of ketones and tertiary alcohols, cyanidation, dichloromethyl ether reaction, Matteson’s Boronnic Ester homologation, Brown’s asymmetric Crotylboration.
Organosilicon reagents: preparation and reactions of alkynylsilanes, alkenylsilanes and allylsilanes. Acyilsilanes,

Reference
3. ROC Norman and Coxon, Principles of Organic Synthesis

Unit 5: Retro synthetic Analysis
Basic principles and terminology of retrosynthesis, synthesis of aromatic compounds, one group and two group C-X disconnections, one group C-C and two group C-C disconnections, amine and alkene synthesis, important strategies of retrosynthesis. Functional group transposition, important functional group interconversions.

Reference

Unit 6: Principles of asymmetric synthesis

Conditions for stereoselectivity: Symmetry and transition state criteria, kinetic and thermodynamic control. Techniques for determination of enantiomeric excess, specific rotation, Chiral NMR; Chiral derivatizing agents, Chiral solvent, Chiral shift reagents and Chiral HPLC.

Reference

1. Stereochemistry of organic compounds — Principles & Applications by D Nasipuri
2. Stereochemistry of Carbon compounds by Ernest L Eliel & Samuel H. Wilen
3. Stereochemistry: Conformation & Mechanism by P S Kalsi

General Reference for Units 1 & 2

Unit 1: Chemical Kinetics

1.1 Theories of reaction rates: Collision theory-steric factor, potential energy surfaces. Conventional transition state theory-Eyring equation. Comparison of the two theories. Thermodynamic formulation of the two theories. Thermodynamic formulation of the reaction rates. Significance of $\Delta G^\ne$, $\Delta H^\ne$ and $\Delta S^\ne$. Volume of activation. Effect of pressure and volume on velocity of gas reactions.

1.2 Lindemann-Hinshelwood mechanism, qualitative idea of RRKM theory, chain reactions: free radical and chain reactions, steady state treatment, kinetics of $\text{H}_2\text{-Cl}_2$ and $\text{H}_2\text{-Br}_2$ reactions, Rice-Herzfeld mechanism, branching chains $\text{H}_2\text{-O}_2$, Semonov-Hinshelwood mechanism of explosive reactions, mechanisms of step growth, ionic and addition polymerization, kinetics of anionic and cationic polymerization.

1.3 Fast reactions: relaxation, flow and shock methods, flash photolysis, NMR and ESR methods of studying fast reactions.

1.4 Reactions in solution: factors determining reaction rates in solutions, effect of dielectric constant and ionic strength, cage effect, Bronsted-Bjerrum equation, primary and secondary kinetic salt effect, influence of solvent on reaction rates, significance of volume of activation, linear free energy relationship, kinetic isotope effect.

1.5 Acid-base catalysis: specific and general catalysis, Skrabal diagram, Bronsted catalysis law, prototropic and protolytic mechanism with examples, acidity function.

1.6 Enzyme catalysis and its mechanism, Michelis-Menten equation, effect of pH and temperature on enzyme catalysis.

Unit 2: Surface Chemistry

2.1 Different types of surfaces, thermodynamics of surfaces, Gibbs adsorption equation and its verification, surfactants and micelles, surface films, surface pressure and surface potential and their measurements and interpretation. Application of low energy electron diffraction and photoelectron spectroscopy, ESCA and Auger electron spectroscopy, scanning probe microscopy, ion scattering, SEM and TEM in the study of surfaces.

2.2 Adsorption: The Langmuir theory, kinetic and statistical derivation, multilayer adsorption-BET theory, Use of Langmuir and BET isotherms for surface area determination.

2.3 Colloids: Zeta potential, electrokinetic phenomena, sedimentation potential and streaming potential, Donnan membrane equilibrium.

2.4 Macromolecules: different averages, methods of molecular mass determination, osmotic, viscosity, sedimentation and light scattering methods.

2.5 Surface Enhanced Raman Scattering, surfaces for SERS studies, chemical enhancement mechanism, surface selection rules, spectrum of 2-aminophenol, applications of SERS.

2.6 Mechanisms of heterogeneous catalysis: unimolecular and bimolecular surface reactions, mechanisms of catalyzed reactions like ammonia synthesis, Fischer-Tropsch reactions, hydrogenation of ethylene and catalytic cracking of hydrocarbons and related reactions.

**Unit 3: Photochemistry (18 hours)**

3.1 Fundamentals of photochemistry: quantum yield, chemical actinometry, excimers, exciplexes, E-type and P-type fluorescence, short range and long range energy transfer, quenching and sensitization.


3.3 Photochemical techniques: flash photolysis, femtosecond transition state spectroscopy, lasers in photochemistry - two-photon spectroscopy, fluorescence imaging methods, radiation chemistry - pulse radiolysis, hydrated electron, chemiluminescence and its analytical applications.

3.4 Solar energy utilization and storage, solar cell and its working, photochemistry of environment, greenhouse effect, photochemistry of vision and nucleic acids, photography, photochromism.

**Reference**


AMCH312: ORGANIC SPECTROSCOPY

Credits: 3
Contact Lecture Hours: 54

Unit 1: Ultraviolet-Visible and Chirooptical Spectroscopy (9 hours)
1.1 Energy levels and selection rules, Woodward-Fieser and Fieser-Kuhn rules.
1.2 Influence of substituent, ring size and strain on spectral characteristics. Solvent effect, Stereochemical effect, non-conjugated interactions. Chirooptical properties-ORD, CD, octant rule, axial haloketone rule, Cotton effect.
1.3 Problems based on the above topics.

Unit 2: Infrared Spectroscopy (9 hours)
2.1 Fundamental vibrations, characteristic regions of the spectrum (fingerprint and functional group regions), influence of substituent, ring size, hydrogen bonding, vibrational coupling and field effect on frequency, determination of stereochemistry by IR technique.
2.2 IR spectra of C=C bonds (olefins and arenes) and C=O bonds.
2.3 Problems on spectral interpretation with examples.

Unit 3: Nuclear Magnetic Resonance Spectroscopy (18 hours)
3.1 Magnetic nuclei with special reference to $^1$H and $^{13}$C nuclei. Chemical shift and shielding/deshielding, factors affecting chemical shift, relaxation processes, chemical and magnetic non-equivalence, local diamagnetic shielding and magnetic anisotropy. $^1$H and $^{13}$C NMR scales.
3.2 Spin-spin splitting: AX, AX2, AX3, A2X3, AB, ABC, AMX type coupling, first order and non-first order spectra, coupling constant, mechanism of coupling, Karplus curve, quadrupole broadening and decoupling, diastereomeric protons, virtual coupling, long range coupling, NOE, Solomon diagram, NOE and cross polarization.
3.3 Simplification non-first order spectra to first order spectra: shift reagents, spin decoupling and double resonance, off resonance decoupling. Chemical shifts and homonuclear/heteronuclear couplings. Basis of heteronuclear decoupling.
3.4 2D NMR and COSY, HOMOCOSY and HETEROCOSY
3.5 Polarization transfer: SPT, Selective Population Inversion, DEPT, INEPT, MRI.
3.6 Problems on spectral interpretation with examples.
Unit 4: Mass Spectrometry (9 hours)

McLafferty rearrangement and its applications. HRMS, MS-MS, LC-MS, GC-MS.

4.2 Problems on spectral interpretation with examples.

Unit 5: Structural Elucidation Using Spectroscopic Techniques (9 hours)

5.1 Identification of structures of unknown organic compounds based on the data from UV-Vis, IR, $^1$H NMR and $^{13}$C NMR spectroscopy (HRMS data or Molar mass or molecular formula may be given).

5.2 Interpretation of the given UV-Vis, IR and NMR spectra

Reference

SEMESTER IV

ELECTIVE COURSES
(Any three courses to be opted from the following courses)

AMCH4E01: ADVANCED INORGANIC CHEMISTRY

Credits: 4  Contact Lecture Hours: 90

Unit 1: Applications of Group Theory  (27 hours)
1.1 Transformation properties of atomic orbitals, hybridization schemes for sigma and pi bonding with examples, Symmetry Adapted Linear Combination of Atomic orbitals in tetrahedral, octahedral and sandwich complexes.
1.2 Ligand field theory-splitting of d orbitals in different environments using group theoretical considerations, construction of energy level diagrams, correlation diagrams, method of descending symmetry, formation of symmetry adapted group of ligands, MO diagrams, splitting terms for orbitals, energy levels, d-d transition-selection rules, vanishing integrals. Raman spectra of complexes with oxo anions as ligands, IR and Raman spectra using character tables in tetrahedral, octahedral and square planar complexes.

Unit 2: Inorganic Spectroscopic Methods  (9 hours)
2.1 Infrared and Raman Spectroscopy: structural elucidation of coordination compounds containing the following molecules/ions as ligands-NH₃, H₂O, CO,NO, OH⁻, SO₄⁻², CN⁻, SCN⁻, NO₂⁻ and X⁻ (X=halogen).
2.2 Electron Paramagnetic Resonance Spectroscopy: EPR of d¹ and d⁹ transition metal ions in cubic and tetragonal ligand fields, evaluation of g values and metal hyperfine coupling constants.
2.3 Mössbauer Spectroscopy: applications of Mössbauer spectroscopy in the study of Fe(III) complexes.

Unit 3: Inorganic Photochemistry  (9 hours)
3.1 Excited states, ligand field states, charge-transfer states and Thexi states, phosphorescence and fluorescence. Photochemical reactions-substitution and redox reactions of Cr(III), Ru(II) and Ru(III) complexes. Applications-synthesis and catalysis, chemical actinometry and photochromism. Metal-metal multiple bonds.
3.2 Metal complex sensitizers-electron relay, semiconductor supported metal oxide systems, water photolysis, nitrogen fixation and CO₂ reduction.

**Unit 4: Nanomaterials** (18 hours)

4.1 General introduction to nanomaterials and emergence of nanotechnology, Moore’s law, synthesis and properties of fullerenes, graphenes, graphynes and carbon nanotubes, synthesis of nanoparticles of gold, silver, rhodium, palladium and platinum, techniques of synthesis-electroplating and electrophoretic deposition, conversion through chemical reactions and lithography. Thin films-chemical vapor deposition and atomic layer deposition techniques.


4.3 Evolving interfaces of nanotechnology-nanobiology, nanosensors, nanomedicines.

**Unit 5: Analytical Methods** (18 hours)

5.1 The basis and procedure of sampling-crushing and grinding, gross sampling. Sampling of solids, liquids, gas, particulate solids, metals and alloys. Preparation of a laboratory sample. Moisture in samples-essential and non essential water, occluded water. Determination of water in samples-direct and indirect methods.

5.2 Decompositions and dissolution-reagents for decomposition and dissolution like HCl, H₂SO₄, HNO₃, HClO₄ and HF. Microwave decompositions, combustion methods. Uses of fluxes like Na₂CO₃, Na₂O₂, KNO₃, K₂S₂O₇, NaOH, B₂O₃ and lithium meta borate.

5.3 Elimination of interferences from samples by precipitation, electrolytic precipitation, separation by extraction and ion exchange separation.

5.4 Analytical procedures involved in the environmental monitoring of water quality-BOD, COD, DO, nitrite and nitrate, iron, fluoride, soil moisture, salinity, soil colloids, cation and anion exchange capacity. Air pollution monitoring: sampling and collection of air pollutants-SO₂, NO₂, NH₃, O₃, and SPM.

**Unit 6: Acids and Bases and Non-aqueous Solvents** (9 hours)

6.1 Acid base concept in non aqueous media-HSAB concept, solvent effects, linear free energy relationship-mechanism and methods of determination.

solvents, non-ionizable polar solvents, polar solvents undergoing autoionization, liquid halogens, inter-halogen compounds, oxy halides, dinitrogen tetroxide, sulphur dioxide.

Reference

AMCH4E02: ADVANCED ORGANIC CHEMISTRY

Credits: 4
Contact Lecture Hours: 90

Unit 1: Metathesis and other reactions

Mechanism of various metathesis reactions, Grubbs 1st, 2nd and 3rd generation catalysts. Hoveyda-Grubbs 1st and 2nd generation catalysts, Schrock-Hoveyda chiral olefien metathesis, Furstner’s alkyne metathesis- synthetic applications of olefien, enyne, alkyne and cross metathesis.
Extrusion reactions- Storey synthesis, azo, S, sulphonyl, CO2, CO extrusion reactions.
Dyotropic rearrangements, Noncyclic rearrangement, Chapman rearrangement, Wallach rearrangement, Reference:


Unit 2: Synthetic Strategies & Research

Tandem, domino, multicomponent, remote functionalisation reactions. One pot synthesis, Green organic synthesis- twelve principles of green chemistry, microwave assisted synthesis, ultra sound assisted synthesis. Click reactions, Combinatorial Synthesis. Synthesis of metallocenes, non benzenoid aromatics and polycyclic aromatic compounds. Basic concepts of research methodology- writing a thesis/dissertation. Literature sources in chemistry.
General structure of a research paper.
Organic Chemistry research developments during last 10 years.

Reference:

Unit 3: Methodologies in asymmetric synthesis (18 hours)


3.2 Chiral Substrate controlled asymmetric synthesis: Nucleophilic additions to chiral carbonyl compounds. 1, 2- asymmetric induction, Cram’s rule and Felkin-Anh model, Cram’s chelate model etc. Diastereoselective aldol reaction (chiral enolate & achiral aldehydes and achiral enolate & chiral aldehydes) its explanation by Zimmerman-Traxel model.

3.3 Chiral auxiliary controlled asymmetric synthesis: α-Alkylation of chiral enolates, imines and hydrazones. 1, 4-Asymmetric induction and Prelog’s rule. Use of chiral auxiliaries in Diels-Alder reaction. Evan’s Assymetricalaldol condensation reaction.

3.4 Chiral reagent controlled asymmetric synthesis: Asymmetric reductions using BINAL-H and CBS reagents. Asymmetric hydroboration using Ipc₂BH and IpcBH₂

Chiral catalyst controlled asymmetric synthesis: Sharpless asymmetric epoxidation, Jacobsen epoxidation, Sharpless asymmetric dihydroxylation, aminohydroxylation, Noyori asymmetric hydrogenation.

3.5 Asymmetric organocatalysis-Proline catalysed aldol reactions, Shi epoxidation, Intramolecular Michael addition reaction by Imidazolidinone catalysts. Enzyme mediated enantioselective synthesis.

Reference

1. Designing of organic synthesis – S. Warren (Wiley)
5. Strategic Applications of named reactions in organic synthesis-Laszlo Kurti and Barbara Czako.

**Unit 4: Supramolecular Chemistry** (9 hours)

Concept of molecular recognition, host-guest complex formation, forces involved in molecular recognition. Molecular receptors(gross structural features only; synthesis not expected): cyclodextrins, crown ethers, cryptands, spherands, tweezers, carcerands, cyclophanes, calixarenes,

Importance of molecular recognition in biological systems like DNA and protein. Targeted drug delivery.

**Reference:**


**Unit 5: Medicinal Chemistry** (9 hours)

Unless otherwise stated, synthesis of the drugs is not expected.

Development of a drug, Drugs, theories of drug action like drug-receptor theory, occupancy theory, induced fit theory, activation- aggression theory. Steps of drug action (selectivity, administration, absorption, binding, excretion etc).

LD50, ED50, therapeutic index, agonist and antagonists. Drug SAR and QSAR.

Important chemicals used in drug action- Sulpha drugs, analgesics, anti pyretics, anti histamines, cardiovascular agents, anti tubercular drugs, antimalarial drugs, anti HIV drugs and anticancer drugs. Central nervous system acting drugs- Types, mode of action and examples.

Antibiotics - Classification, classical antibiotics like penicillin, chloramphenicol, tetracycline, streptomycin, cephalosporins.

Modern antibiotics- semisynthetic penicillin, ammoxylin, ampicillin, erythromycin, azithromycin, ceftrudoxime, cefexime etc. (uses and advantages only, structural features not required)

Polyene antifungal antibiotics-nystatin, fusicidic acid-griesofulvin. (gross structural features not needed).
Reference:
3. Bentley and Drivers' TB of Pharmaceutical Chemistry.
4. Graham Patrick, Medicinal Chemistry, Garland Science

Unit 7: Synthesis of carbocyclic rings (9 hours)
7.1 Different approaches towards the synthesis of three, four, five and six-membered rings. Photochemical approaches for the synthesis of four membered rings-oxetanes and cyclobutanes, ketene cycloaddition (inter and intra molecular), Pauson-Khand reaction, Volhardt reaction, Bergman cyclization, Nazarov cyclization, cation-olefin cyclization.
7.2 Inter-conversion of ring systems (contraction and expansion)-Demjenov reaction, Reformatsky reaction. Construction of macrocyclic rings-ring closing metathesis.
7.3 Inter and Intramolecular Paterno-Buchi reaction: synthetic applications (at least four) e.g. in the preparation of Azulene. Synthetic applications (at least four each) of RCM (ring closing metathesis) and ROMP (ring – opening metathesis polymerization) Synthetic utility of Diels – Alder reaction in the preparation of Ibogamine (antitumour alkaloid) and reserpine

Reference:

Unit 8: Natural Products (18 hours)
8.2 Proteins, DNA and RNA- structure, methods for primary structure determination of peptides, proteins and nucleic acids. Replication of DNA, protein biosynthesis, transcription and translation.

8.3 Forward synthesis of nuciferal, longifolene, luciferin, Corey lactone and prostogladins, 11α-hydroxyprogesterone, camphor, atropine, papaverine, quinine, cyanin, quercetin, β-carotene, testosterone, PGE₂ and PGF₂α, camphor, Vitamin D, Juabione. Inter-conversions of steroids.

8.4 Basic principles of the biosynthesis of terpenes, steroids, alkaloids, carbohydrates, proteins and nucleic acids. Biosynthesis of cholesterol, morphine and phenyl alanine. Biomimetic synthesis of progesterone and spatreine.

Reference
1. IL Finar Organic Chemistry, Vol 1 & 2

Unit 9: Polymers (9 hours)

Reference
Unit 1: Computational Chemistry (27 hours)

1.1 Introduction: Fields of application; Basics of Different methods: Ab initio, Density functional, Semi-empirical, Molecular Mechanics and Molecular Dynamics, Comparison of their performance; Potential Energy Surfaces: Stationary points, saddle point, local and global minima, their significance. Examples: PES for water, PES for ozone-isoozone interconversion.

1.2 Molecular Mechanics: Concept of Force Field, its components for bond stretching, bending, torsional motion, non-bonded and electrostatic interactions, cross-terms and valence-terms, parameterization of each of them, Examples for force fields: MM2, AMBER and CHARMM. Molecular Mechanics: Areas of application.

1.3 Molecular Dynamics: General Principles of MD simulations, Ingredients of MD simulations: potentials in MD simulation and boundary conditions; algorithm for molecular dynamics. Application and limitation of MD.

1.4 Ab initio Quantum Methods: Concept of Basis Sets, types and nomenclature; Slater and Gaussian functions; Hartree-Fock Methods: Basic concepts for Hartree-Fock (HF), Restricted open-shell Hartree-Fock (ROHF) and Unrestricted Hartree-Fock (UHF) methods; Introduction to post-Hartree-Fock methods: Möller-Plesset perturbation theory, Configuration Interaction (CI), Coupled Cluster (CC), Quadratic Configuration Interaction. Semi-empirical Quantum Chemistry Methods: Basic Concepts. Density Functional Methods: General Principles, Hohenberg-Kohn theorem, Kohn-sham model (derivations not expected).

1.5 Chemical Computations: Molecular geometry, Cartesian coordinates, internal coordinates, z-matrix, construction of z-matrix with examples. Calculations using GAMESS/Gaussian: setting basis set, method, charge and multiplicity; programs for single point energy calculations, geometry optimization, constrained optimization and frequency calculations; Practice to locate local minima, saddle points and transitions states; calculation of enthalpies of reaction, conformational analysis (ethane) Calculation of ionization energy, electron affinity and atomic charges of known systems using Koopman’s theorem; Identification of HOMO and LUMO.
Unit 2: Diffraction Methods and Atomic Spectroscopic Techniques (9 hours)

2.2 Atomic absorption spectroscopy (AAS), principle of AAS, absorption of radiant energy by atoms, classification of atomic spectroscopic methods, measurement of atomic absorption, instrumentation.
2.3 Atomic emission spectroscopy (AES), advantages and disadvantages of AES, origin of spectra, principle and instrumentation.
2.4 Flame emission spectroscopy (FES), flames and flame temperature, spectra of metals in flame, instrumentation.

Unit 3: Fluorescence Spectroscopy (9 hours)

3.1 Characteristics of fluorescence emission, lifetime, quantum yield, quenching, resonance energy transfer, time resolved fluorescence
3.2 Basic Instrumentation: light source, monochromator, optical filters, photomultiplier tube, polarizers.
3.3 Fluorescence sensing, mechanism of sensing, sensing techniques based on collisional quenching, energy transfer and electron transfer, examples of pH sensors. Novel fluorephores: long life time metal-ligand complexes.

Unit 4: Electrochemistry and Electromotive Force (27 hours)

4.1 Theories of ions in solution, Drude and Nernst’s electrostriction model and Born’s model, Debye-Huckel theory, Derivation of Debye-Huckel-Onsager equation, validity of DHO equation for aqueous and non aqueous solutions, Debye- Falkenhagen effect, conductance with high potential gradients, activity and activity coefficients in electrolytic solutions, ionic strength, Debye-Huckel limiting law and its various forms, qualitative and quantitative tests of Debye-Huckel limiting equation, deviations from the DHLL. Osmotic coefficient, ion association, fraction of association, dissociation constant, triple ion and conductance minima, equilibria in electrolytes, association constant, solubility product principle, solubility in presence of common ion, instability constant, activity coefficient and solubility measurement, determination of activity coefficient from equilibrium constant measurement.
4.2 Electrochemical cells, concentration cells and activity coefficient determination, liquid junction potential, evaluation of thermodynamic properties, the electrode double layer,
electrode-electrolyte interface, different models of double layer, theory of multilayer capacity, electrocapillary, Lippmann equation, membrane potential.

4.3 Fuel cells, classification based on working temperature, chemistry of fuel cells, H2-O2 fuel cells.

4.4 Polarization - electrolytic polarization, dissolution and decomposition potential, concentration polarization, overvoltage, hydrogen and oxygen overvoltage, theories of overvoltage, Tafel equation and its significance, Butler-Volmer equation for simple electron transfer reactions, transfer coefficient, exchange current density, rate constants.

**Unit 5: Electroanalytical Techniques** (18 hours)

5.1 Voltametry and polarography: Voltametry-cyclic voltametry, ion selective electrodes, anodic stripping voltametry. Polarography-decomposition potential, residual current, migration current, supporting electrolyte, diffusion current, polarogram, half wave potential, limiting current density, polarograph, explanation of polarographic waves.

5.2 The dropping mercury electrode, advantages and limitations of DME, applications of polarography, quantitative analysis- pilot ion procedure, standard addition methods, qualitative analysis-determination of half wave potential of an ion, advantages of polarography.

5.3 Amperometric titrations: general principles of amperometry, application of amperometry in the qualitative analysis of anions and cations in solution, instrumentation, titration procedure, merits and demerits of amperometric titrations.

5.4 Coulometry: coulometer-Hydrogen Oxygen coulometers, silver coulometer, coulometric analysis with constant current, coulometric tritrations, application of coulometric titrations-neutralization titrations, complex formation titrations, redox titrations. Advantages of coulometry.

**Reference**

8. S. Glasstone, Introduction to Electrochemistry, Biblio Bazar, 2011
17. J.P. Fackler Jr., L.R. Falvello (Eds.), Techniques in Inorganic Chemistry: Chapter 4, CRC Press, 2011.
SEMESTERS III AND IV

PRACTICAL

AMCH4P04: INORGANIC CHEMISTRY PRACTICAL - II

Credits: 3  Contact Lab Hours: 54+54 =108

PART I
Estimation of simple binary mixtures (like Cu-Ni, Cu-Zn, Fe-Cr, Fe-Cu, Fe-Ni, Pb-Ca) of metallic ions in solution by volumetric and gravimetric methods.

PART II
Analysis of one of the alloys of brass, bronze and solder. Analysis of one of the ores from hematite, chromite, dolomite, monazite, ilmenite.

Reference
AMCH4P05: ORGANIC CHEMISTRY PRACTICAL – II

Credits: 3

Contact Lab Hours: 54+54=108

1. Three Stage Synthesis (some examples)
   1. Anthranilic acid – o-chlorobenzoic acid- N-phenylantranilic acid- acridone
   2. O-toludine- o-chlorotoluene- o-chlorobenzoic acid- N-phenylantranilic acid
   3. Nitrobenzene- aniline- tribromoaniline- symm- tri bromobenzene
   4. Benzene- nitrobenzene- hydrazobenzene- benzidine (benzidine rearrangement)
   5. Nitrobenzene- meta dinitrobenzene- m-nitroaniline- m-phenylenediamine
   6. Benzene- nitrobenzene- azoxybenzene- azobenzene
   7. Benzene- nitrobenzene- phenylhydroxylamine- p-aminophenol
   8. Benaldehyde- benzoin- benzyl- benzilic acid
   9. Clorobenzene- 1-chloro 2,4- dinitrobenzene – 2,4-dinitrophenol- picric acid
  10. Phthalic anhydride- o-benzoylebenzoic acid- anthraquinone- anthrone

(3 stage synthesis can be a combination of conventional, green, microwave assisted or sonochemical reactions)

(Minimum 7 preparations to be done in the lab)

2. Microwave Assisted Organic Reactions & Green Chemistry Synthesis (Minimum 7)
4. TLC of organic binary mixtures with an aim to find to separate them by finding the solvent mixture for separation.
5. Quantitative separation of typical binary mixture using column chromatography.
6. Physical organic chemistry experiments

Final product of the synthesis shall be exhibited during examination.

Reference:


I Chemical Kinetics
1. Determination of the rate constant of the hydrolysis of ester by acid.
2. Kinetics of reaction between K2S2O8 and KI

II Polarimetry
1. Kinetics of the inversion of sucrose in presence of HCl.
2. Determination of the concentration of a sugar solution.
3. Determination of the concentration of HCl.
4. Determination of the relative strength of acids.

III Refractometry
1. Identification of pure organic liquids and oils.
2. Determination of molar refractions of pure liquids.
3. Determination of concentration of solutions (KCl-water, glycerol-water)
4. Determination of molar refraction of solids.
5. Study of complex formation between potassium iodide and mercuric iodide system.

IV Conductivity measurements
1. Verification of Onsager equation.
2. Determination of the degree of ionization of weak electrolytes.
3. Determination of pKa values of organic acids.
4. Titration of a mixture of acids against a strong base.
5. Titration of a dibasic acid against a strong base.

V Potentiometry
1. Titration of a mixture of acids against a strong base.
2. Determination of the concentration of a mixture of Cl⁻ and I⁻ ions.

Reference
Part B

Computational chemistry experiments

Experiments illustrating the capabilities of modern paid/ open source/free computational chemistry packages in computing single point energy, geometry optimization, vibrational frequencies, population analysis, conformational studies, IR and Raman spectra, transition state search, molecular orbitals, dipole moments etc.

Geometry input using Z-matrix for simple systems, obtaining Cartesian coordinates from structure drawing programs like Chemsketch.

Reference

5. Gaussian www.gaussian.com