DEPARTMENT OF
CHEMISTRY

Curriculum and Syllabus for Postgraduate Programme in Polymer Chemistry Under Credit Semester System (with effect from 2019 admissions)

St Berchmans College
Founded 1922
AUTONOMOUS | College with Potential for Excellence | Reaccredited by NAAC with A Grade
Affiliated to Mahatma Gandhi University, Kottayam, Kerala
Changanassery, Kottayam, Kerala, India-686101

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20.	Dr. Renchu Scaria	Assistant Professor Department of Chemistry St Berchmans College, Changanassery
21.	Mrs. Sajini T	Assistant Professor Department of Chemistry St Berchmans College, Changanassery

Programme Objectives

- To provide a broad foundation in the latest developments in chemistry that enables scientific reasoning and analytical problem solving.
- To achieve the skills required to succeed in research areas and in chemical industry.
- To familiarise with modern instrumentation methods.
- To develop the ability to communicate scientific information and research results to the society
- To learn the laboratory skills required to design and interpret the chemical information.
- Introduction of necessary skills for synthesis, separation and characterisation of compounds using laboratory and instrumentation techniques.
- To help in understanding the environmental issues
- Enables to understand latex technology.
- Enables to understand dry rubber technology.
- Enables to understand plastic technology.

Programme Outcome

- Capacity to interpret various issues related to scientific developments in terms of chemical terminology.
- Exposure to handle modern instruments such as UV, IR, AAS.....etc.
- Expertise in laboratory techniques.
- Expertise appropriate techniques for the qualitative and quantitative analysis.
- Aware of the environmental issues related to plastic waste.
- Necessity of recycling process.
- understand latex technology.
- understand dry rubber technology.
- understand plastic technology.

REGULATIONS FOR POSTGRADUATE (PG) PROGRAMMES UNDER CREDIT SEMESTER SYSTEM (SB-CSS-PG) 2019

1. SHORT TITLE

1.1 These Regulations shall be called St. Berchmans College (Autonomous) Regulations (2019) governing postgraduate programmes under Credit Semester System (SB-CSS-PG).

1.2 These Regulations shall come into force with effect from the academic year 2019 - 20 onwards.

2. SCOPE

2.1 The regulation provided herein shall apply to all regular postgraduate programmes, MA/MSc/MCom, conducted by St. Berchmans College (Autonomous) with effect from the academic year 2019 - 20.

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 SB-CSS-PG system.

3.4 'Academic Council' means the Committee consisting of members as provided under section 107 of the University Act 2014, Government of Kerala.

3.5 'Parent Department' means the Department, which offers a particular postgraduate programme.

3.6 'Department Council' means the body of all teachers of a Department in the College.

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 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 a postgraduate programme shall be four (4) semesters.

3.10 'Semester' means a term consisting of a minimum 90 working days, inclusive of tutorials, examination days and other academic activities within a period of six months.

3.11 'Course' means a segment of subject matter to be covered in a semester. Each Course is to be designed under lectures/tutorials/laboratory or fieldwork/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 respective Board of Studies.

3.15 The elective course shall be either in the fourth semester or be distributed among third and fourth semesters.

3.16 'Audit Course' means a course opted by the students, in addition to the compulsory courses, in order to develop their skills and social responsibility.

3.17 'Extra Credit Course' means a course opted by the students, in addition to the compulsory courses, in order to gain additional credit that would boost the performance level and additional skills.

3.18 Extra credit and audit courses shall be completed by working outside the regular teaching hours.

3.19 There will be optional extra credit courses and audit courses. The details of the extra credit and audit courses are given below.

Semester	Course	Type
I	Course on Mendeley Reference Management Software	Optional, Extra credit Grades shall be given
	Course on Basic Life Support System and Disaster Management	Compulsory, Audit Grades shall be given
First summer vacation	Internship/Skill Training	Optional, Extra credit Grades shall be given
Any time during the programme	Oral Presentation in National/International seminar	Optional, Extra credit
	Publication in a recognized journal with ISSN number	

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

3.21 'Dissertation' means a minor thesis to be submitted at the end of a research work carried out by each student on a specific area.

3.22 'Plagiarism' is the unreferenced use of other authors' material in dissertations and is a serious academic offence.

3.23 '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.

3.24 '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.

3.25 'Improvement Examination' is an examination conducted to improve the performance of students in the courses of a particular semester.

3.26 'Supplementary Examination' is an examination conducted for students who fail in the courses of a particular semester.

3.27 The minimum credits, required for completing a postgraduate programme is eighty (80).

3.28 'Credit' (C) of a course is a measure of the weekly unit of work assigned for that course in a semester.

3.29 '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.

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

3.31 'Grade Point' (GP) is the numerical indicator of the percentage of marks awarded to a student in a course.

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

3.33 'Semester Grade Point Average' (SGPA) 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.

3.34 'Cumulative Grade Point Average' (CGPA) 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.

3.35 'Institution average' is the value obtained by dividing the sum of the marks obtained by all students in a particular course by the number of students in respective course.

3.36 '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.

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

3.38 First, Second and Third position shall be awarded to students who come in the first three places based on the overall CGPA secured in the programme in the first chance itself.

4. PROGRAMME STRUCTURE

4.1 The programme shall include two types of courses; Core Courses and Elective Courses. There shall be a project/research work to be undertaken by all students. The programme will also include assignments, seminars, practical, viva-voce etc., if they are specified in the curriculum.

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

4.3 **Project/dissertation**

Project/research work shall be completed by working outside the regular teaching hours except for MSc Computer Science programme. Project/research work 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 in an industrial/research organization on the recommendation of the supervisor. There shall be an internal assessment and external assessment for the project/dissertation. The external evaluation of the Project/Dissertation shall be based on the individual presentation in front of the expert panel.

4.4 **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 all courses.

4.5 **In-semester assessment of theory courses**

The components for ISA are given below.

Component	Marks
Attendance	2
Viva	3
Assignment	4
Seminar	4
Class test	4
Model Exam	8
Total	**25**

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

% of Attendance	Marks
Above 90	2
75 – 90	1

4.7 **Assignments**

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

4.8 **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.

4.9 **In-semester examination**

Every student shall undergo at least two in-semester examinations - one as class test and second as model examination as internal component for every theory course.

4.10 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 course teacher and 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 shall be kept in the office of the Head of the Department for at least two years for verification.

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

The internal assessment of practical courses shall be conducted either annually or in each semester. There shall be one in-semester examination for practical courses. The examination shall be conducted annually or in each semester. The components for internal assessment is given below.

Component	Marks
Attendance	2
Lab Test	15
Viva-Voce	5
Record	3
Total	**25**

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

% of Attendance	Marks
Above 90	2
75 - 90	1

4.12 **End-semester assessment**

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

4.13 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.

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

4.15 A question paper may contain short answer type/annotation, short essay type questions/problems and long essay type questions. Marks for each type of question can vary from programme to programme, but a general pattern may be followed by the Board of Studies.

4.16 Question Pattern for external theory examination shall be,

Science and Commerce

Section	Total No. of Questions	Questions to be Answered	Marks	Total Marks for the Section
A	14	10	2	20
B	8	5	5	25
C	4	2	15	30
			Maximum	**75**

4.17 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.

4.18 Practical examination shall be conducted annually or in each semester. Practical examination shall be conducted by one external examiner and one internal examiner. The question paper setting and evaluation of answer scripts shall be done as per the directions in the examination manual of the College. The duration of practical examination shall be decided by the Board of Studies.

4.19 Project/Dissertation evaluation shall be conducted at the end of the programme. Project/Dissertation evaluation shall be conducted by one external examiner and one internal examiner. The components and mark division for internal and external assessment shall be decided by the respective Board of Studies.

Components of Project Evaluation	**Marks**
Internal Evaluation	25
Dissertation (External)	50
Viva-Voce (External)	25
Total	**100**

4.20 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).

4.21 For all courses (theory and practical) an indirect grading system based on a seven (7) 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.

Percentage of Marks	**Grade**	**Performance**	**Grade Point**
95 and above	S	Outstanding	10
85 to below 95	A+	Excellent	9
75 to below 85	A	Very Good	8
65 to below 75	B+	Good	7
55 to below 65	B	Above Average	6
45 to below 55	C	Satisfactory	5
40 to below 45	D	Pass	4
Below 40	F	Failure	0

4.22 **Credit Point**

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

$$\mathbf{CP = C \times GP}$$

where C is the credit and GP is the grade point

4.23 **Semester Grade Point Average**

Semester Grade Point Average (SGPA) is calculated using the formula

$$\mathbf{SGPA = TCP/TCS}$$

where TCP is the total credit point of all the courses in the semester and TCS is the total credits in the semester

GPA shall be rounded off to two decimal places.

4.24 **Cumulative Grade Point Average**

Cumulative Grade Point Average (CGPA) is calculated using the formula

CGPA = TCP/TC

where TCP is the total credit point of all the courses in the whole programme and TC is the total credit in the whole programme

GPA shall be rounded off to two decimal places.

Grades for the different courses, semesters, Semester Grade Point Average (SGPA) and grades for overall programme, Cumulative Grade Point Average (CGPA) are given based on the corresponding Grade Point Average (GPA) as shown below:

GPA	Grade	Performance
9.5 and above	S	Outstanding
8.5 to below 9.5	A+	Excellent
7.5 to below 8.5	A	Very Good
6.5 to below 7.5	B+	Good
5.5 to below 6.5	B	Above Average
4.5 to below 5.5	C	Satisfactory
4 to below 4.5	D	Pass
Below 4	F	Failure

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

5. SUPPLEMENTARY/IMPROVEMENT EXAMINATION

5.1 There will be supplementary examinations and chance for improvement. Only one chance will be given for improving the marks of a course.

5.2 There shall not be any improvement examination for practical courses and examinations of the final year.

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. This condonation shall not be counted for internal assessment.

6.2 Benefit of attendance may be granted to students representing 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 etc., on production of participation/attendance certificates, within one week from competent authorities, for the actual number of days participated, subject to a maximum of ten (10) days in a semester, 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 in 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 after readmission.

7. BOARD OF STUDIES AND COURSES

7.1 The Board of Studies concerned shall design all the courses offered in the programme. The Board 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 programme shall contain programme objectives and programme outcome.

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

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

7.5 Every programme conducted under Credit Semester System shall be monitored by the Academic Council.

8. REGISTRATION

8.1 A student who registers his/her name for the external exam for a semester will be eligible for promotion to the next semester.

8.2 A student who has completed the entire curriculum requirement, but could not register for the Semester examination can register notionally, for getting eligibility for promotion to the next semester.

8.3 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

9. ADMISSION

9.1 The admission to all PG programmes 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 an academic and examination calendar prepared by the College for the conduct of the programmes.

10. ADMISSION REQUIREMENTS

10.1 Candidates for admission to the first semester of the PG programme 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.

11. MARK CUM GRADE CARD

11.1 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, SGPA and Letter Grade in the semester
xii. Weighted Average Score
xiii. Result
xiv. Credits/Grade of Extra Credit and Audit Courses

11.2 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 CGPA and the overall letter grade of a student for the entire programme.

11.3 A separate grade card shall be issued at the end of the final semester showing the extra credit and audit courses attended by the student, grade and credits acquired.

12. AWARD OF DEGREE

The successful completion of all the courses with 'D' grade shall be the minimum requirement for the award of the degree.

13. 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.

14. GRIEVANCE REDRESS COMMITTEE

14.1 In order to address the grievance of students relating to ISA, a two-level grievance redress mechanism is envisaged.

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

14.3 Department level: The Principal shall form a Grievance Redress 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 of the students.

14.4 College level: There shall be a College level Grievance Redress 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 of the students.

15. 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.

REGULATIONS FOR EXTRACURRICULAR COURSES, INTERNSHIP AND SKILL TRAINING

COURSE ON BASIC LIFE SUPPORT SYSTEM AND DISASTER MANAGEMENT (BLS & DM)

i. The course on BLS & DM shall be conducted by a nodal centre created in the college.
ii. The nodal centre shall include at least one teacher from each department. A teacher shall be nominated as the Director of BLS & DM.
iii. The team of teachers under BLS & DM shall function as the trainers for BLS & DM.
iv. The team of teachers under BLS & DM shall be given intensive training on Basic Life Support System and Disaster Management and the team shall be equipped with adequate numbers of mannequins and kits for imparting the training to students.
v. Each student shall under go five (5) hours of hands on training in BLS & DM organised by the Centre for BLS & DM.
vi. The training sessions shall be organised on weekends/holidays/vacation during the first semester of the programme.
vii. After the completion of the training, the skills acquired shall be evaluated using an online test and grades shall be awarded.
viii. Nodal centre for BLS & DM shall conduct online test and publish the results.
ix. Students who could not complete the requirements of the BLS & DM training shall appear for the same along with the next batch. There shall be two redo opportunity.
x. For redressing the complaints in connection with the conduct of BLS & DM students shall approach the Grievance Redress Committee functioning in the college.

COURSE ON MENDELY REFERENCE MANAGEMENT SOFTWARE

i. College shall arrange workshop with hands on training in Mendely reference management software during the first semester.
ii. Students completing the course can enrol for an evaluation and those who pass the evaluation shall be given one credit.

INTERNSHIP/SKILL TRAINING PROGRAMME

i. Postgraduate student can undergo an internship for a minimum period of five days (25 hours) at a centre identified by the concerned department. In the case of disciplines where internship opportunities are scanty (e.g. Mathematics) special skill training programmes with duration of five days (25 hours) shall be organised.
ii. Each department shall identify a teacher in charge for internship/skill training programme.
iii. The department shall select institutions for internship/organising skill training programme.
iv. Internship/skill training programme shall be carried out preferably during the summer vacation following the second semester or during the Christmas vacation falling in the second semester or holidays falling in the semester.
v. At the end of the stipulated period of internship each student shall produce an internship completion cum attendance certificate and an illustrated report of the training he/she has underwent, duly certified by the tutor and Head of the institution where the internship has been undertaken.
vi. Students undergoing skill training programme shall submit a training completion cum attendance certificate and a report of the training he/she has underwent, duly certified by the trainer, teacher co-ordinator of the programme from the concerned department and the head of the department concerned.
vii. Upon receipt of the internship completion cum attendance certificate and illustrated report of the training or a training completion cum attendance certificate and a report of the training, the teacher in charge of internship/skill training programme shall prepare a list of students who have completed the internship/skill training programme and a list of students who failed to complete the programme. Head of the department shall verify the lists and forward the lists to the Controller of Examinations.

PAPER PRESENTATION

i. During the period of the programme students shall be encouraged to write and publish research/review papers.
ii. One research/review paper published in a UGC approved journal or oral presentation in an international/national seminar which is later published in the proceedings shall fetch one credit.

VIRTUAL LAB EXPERIMENTS/MOOC COURSES

i. During the tenure of the programme, students shall be encouraged to take up Virtual Lab Experiments and/or MOOC Courses.
ii. College shall arrange dedicated infrastructure for taking up Virtual Lab experiments and/or MOOC courses.
iii. There shall be a Nodal Officer and a team of teachers to coordinate the logistics for conducting Virtual Lab experiments and MOOC courses and to authenticate the claims of the students regarding the successful completion of the Virtual Lab experiments and or MOOC courses.
iv. Students who are desirous to do Virtual Lab experiments and or MOOC courses shall register with the Nodal Officer at the beginning of the experiment session/MOOC course. Students also shall submit proof of successful completion of the same to the Nodal officer.
v. Upon receipt of valid proof, the Nodal Officer shall recommend, to the Controller of Examinations, the award of extra credits. In the case of Virtual Lab experiments, 36 hours of virtual experimentation shall equal one credit and in the case of MOOC courses 18 hours of course work shall equal one credit.

Model Mark cum Grade Card

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MARK CUM GRADE CARD

Date:

Name of the Candidate :

Permanent Register Number (PRN) :

Degree :

Programme :

Name of Examination :

Faculty :

Photo

Course Code	Course Title	Credits (C)	Marks						Grade Awarded (G)	Grade Point (GP)	Credit Point (CP)	Institution Average	Result
			ISA		ESA		Total						
			Awarded	Maximum	Awarded	Maximum	Awarded	Maximum					
	Total SGPA: SG: WAS: ***End of Statement***												

*WAS: Weighted Average Score

Entered by:

Verified by:

Controller of Examinations **Principal**

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Changanassery, Kottayam, Kerala, India - 686101, Tel: 91-481-2420025, 9961231314
E-mail: sbc@sbcollege.org Web: www.sbcollege.ac.in

CONSOLIDATED MARK CUM GRADE CARD

Name of the Candidate :

Permanent Register Number (PRN) :

Degree :

Programme :

Faculty :

Date :

Photo

Course Code	Course Title	Credits (C)	Marks						Grade Awarded (G)	Grade Point (GP)	Credit Point (CP)	Institution Average	Result
			ISA		ESA		Total						
			Awarded	Maximum	Awarded	Maximum	Awarded	Maximum					
SEMESTER I													
SEMESTER II													
SEMESTER III													

SEMESTER IV													
	End of Statement												

PROGRAMME RESULT

Semester	Marks Awarded	Maximum Marks	Credit	Credit Point	SGPA	Grade	WAS	Month & Year of Passing	Result
I II III IV									
Total					**FINAL RESULT: CGPA =**		**; GRADE =**	**;WAS =**	

*** Separate grade card is issued for Audit and Extra Credit courses.**
**** Grace Mark awarded.**

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 seven (7) point scale based on the percentage of Total Marks (ISA + ESA) as given in Table 1. Decimals are corrected to the nearest whole number.

Credit Point and Grade Point Average

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

CP = C × GP

where C is the Credit and GP is the Grade Point

Grade Point Average of a Semester (SGPA) or Cumulative Grade Point Average (CGPA) for a Programme is calculated using the formula

SGPA or CGPA = TCP/TC

where TCP is the Total Credit Point for the semester/programme and TC is the Total Credit for the semester/programme

GPA shall be rounded off to two decimal places.

The percentage of marks is calculated using the formula;

$$\% \text{ Marks} = \left(\frac{\text{total marks obtained}}{\text{maximum marks}}\right) \times 100$$

Weighted Average Score (WAS) is 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.

Percentage of Marks	Grade	Performance	Grade Point
95 and above	S	Outstanding	10
85 to below 95	A+	Excellent	9
75 to below 85	A	Very Good	8
65 to below 75	B+	Good	7
55 to below 65	B	Above Average	6
45 to below 55	C	Satisfactory	5
40 to below 45	D	Pass	4
Below 40	F	Failure	0

Table 1

Grades for the different Semesters and overall Programme are given based on the corresponding GPA, as shown in Table 2.

GPA	Grade	Performance
9.5 and above	S	Outstanding
8.5 to below 9.5	A+	Excellent
7.5 to below 8.5	A	Very Good
6.5 to below 7.5	B+	Good
5.5 to below 6.5	B	Above Average
4.5 to below 5.5	C	Satisfactory
4 to below 4.5	D	Pass
Below 4	F	Failure

Table 2

Note: Course title followed by (P) stands for practical course. A separate minimum of 40% marks each for internal and external assessments (for both theory and practical) and an aggregate minimum of 40% marks is required for a pass in each course. For a pass in a programme, a separate minimum of Grade D for all the individual courses and an overall Grade D or above are mandatory. If a candidate secures Grade F for any one of the courses offered in a Semester/Programme, only Grade F will be awarded for that Semester/Programme until the candidate improves this to Grade D or above within the permitted period.

PROGRAMME STRUCTURE

	Course Code	Course Title	Hours /Week	Total Hours	Credit	ISA	ESA	Total
Semester I	BMCP101	Statistical and Classical Thermodynamics for Polymer Chemistry	3	54	3	25	75	100
	BMCP102	Group Theory and Introductory Quantum Mechanics	4	72	4	25	75	100
	BMCP103	Chemistry of Metal Complexes	4	72	4	25	75	100
	BMCP104	Basic Organic Chemistry for Polymer Chemists	4	72	4	25	75	100
		Inorganic Chemistry Practical - I (P)	3	54	Evaluation at the end of second semester			
		Organic Chemistry Practical - I (P)	3	54				
		Physical Chemistry Practical - 1 (P)	4	72				
		Total	**25**	**450**	**15**	**100**	**300**	**400**
Semester II	BMCP205	Advanced Topics In Theoretical Chemistry	3	54	3	25	75	100
	BMCP206	Principles of Molecular Spectroscopy and Solid State	4	72	4	25	75	100
	BMCP207	Bioinorganic Chemistry, Nuclear Chemistry and Organometallic Compounds	4	72	4	25	75	100
	BMCP208	Physical Organic Chemistry and Organic Reactions	4	72	4	25	75	100
	BMCP2P01	Inorganic Chemistry Practical - I (P)	3	54	3	25	75	100
	BMCP2P02	Organic Chemistry Practical - I (P)	3	54	3	25	75	100
	BMCP2P03	Physical Chemistry Practical - I (P)	4	72	3	25	75	100
		Total	**25**	**450**	**24**	**175**	**525**	**700**
Semester III	BMCP309	Materials Chemistry	4	72	4	25	75	100
	BMCP310	Concepts of Polymer Chemistry	4	72	4	25	75	100
	BMCP311	Physical Chemistry for Polymer Science	4	72	4	25	75	100
	BMCP312	Spectroscopic Methods in Organic Chemistry	3	54	3	25	75	100
		Polymer Preparative Practical (P)	3	54	Evaluation at the end of fourth semester			
		Polymer Characterization Practical (P)	3	54				
		Polymer Processing and Testing Practical (P)	4	72				
		Total	**25**	**450**	**15**	**100**	**300**	**400**
Semester IV	BMCP413	Applied Polymer Science	3	54	3	25	75	100
		Elective Course	4	72	3	25	75	100
		Elective Course	4	72	3	25	75	100
		Elective Course	4	72	3	25	75	100
	BMCP4P04	Polymer Preparative Practical (P)	3	54	3	25	75	100
	BMCP4P05	Polymer Characterization Practical (P)	3	54	3	25	75	100
	BMCP4P06	Polymer Processing and Testing Practical (P)	4	72	3	25	75	100
	BMCP4PJ	Project	-	-	3	25	75	100
	BMCP4VV	Viva-Voce	-	-	2	-	100	100
		Total	**25**	**450**	**26**	**200**	**700**	**900**
		Grand Total	**-**	**-**	**80**	**575**	**1825**	**2400**

ELECTIVE COURSES

Course Code	Course Title
BMCP4E01	Properties and Characterization of Polymers
BMCP4E02	Polymer Science and Technology
BMCP4E03	Synthetic Organic Chemistry
BMCP4E04	Modern Analytical Instrumentation

SEMESTER I

BMCP101: STATISTICAL AND CLASSICAL THERMODYNAMICS FOR POLYMER CHEMISTRY

Credit: 3 **Total Hours: 54**

Objectives

The objective of this course is to make the student aware of

- Working knowledge of laws of thermodynamics
- Applying laws to physical and chemical changes and to biological systems.
- Various types of particles and their distribution in various energy modes
- The correlation of bulk property to particle distribution
- The application of statistical methods for modelling of material properties like heat capacity

Outcome

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

- Derive and discuss the second and third laws of thermodynamics.
- Describe the relationship between different thermodynamic functions at equilibrium conditions
- Explain the driving forces that are responsible for physical, chemical and biological processes
- Understand the statistical distribution of various types of particles in different energy modes
- Calculate partition function and bulk properties
- Apply statistical mechanics for explaining the material properties

Module 1: Aspects of Thermodynamics (18 hours)

1.1 Entropy, dependence of entropy on variables of a system. Thermodynamic equations of state. Irreversible processes - Clausius inequality.

1.2 Free energy and work function, variation of A and with V,T and P, Maxwell relations and significance, temperature dependence of free energy- Gibbs Helmholtz equation, applications of Gibbs Helmholtz equation. Conditions for equilibrium

1.3 Partial molar quantities, chemical potential and Gibbs-Duhem equations

1.4 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, determination of activity.

1.5 Thermodynamics of mixing, Gibbs-Duhem-Margules equation, Konowaloff's rule, Henry's law, excess thermodynamic functions-free energy, enthalpy, entropy and volume.

1.6 Chemical affinity and thermodynamic functions, effect of temperature and pressure on chemical equilibrium- vant Hoff reaction isochore and isotherm.

1.7 Determination of absolute entropies - Nernst heat theorem, Kirchoff's equation. Third law of thermodynamics. Entropy changes in chemical reactions.

1.8 Clapeyron equation and its applications, integrated form. 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.

Textbooks

1. P. W. Atkins, J.de Paula, Physical Chemistry: Thermodynamics, Structure, and Change, 10th Edn., Oxford University Press, 2014
2. R. J. Silbey, R. A. Alberty, M. G. Bawendi, Physical Chemistry, 4th Edn., John Wiley & Sons, 2005
3. J. Rajaram, J.C. Kuriakose, Thermodynamics for Students of Chemistry, 3rd Edn., S Chand and Co; 1999.
4. B. R. Puri, L. R. Sharma, M. S. Pathania, Principles of Physical Chemistry,47th Edn., Vishal Publishing Co., 2018
5. R. P. Rastogi and R. R. Misra, An Introduction to Chemical Thermodynamics, 6thEdn., Vikas Publishing House Pvt. Ltd., 2014

Reference

1. G. W. Castellan, Physical Chemistry, 3rd Edn., Narosa Publishing House, 2004
2. I. N. Levine, Physical Chemistry, 6thEdn., McGraw Hill, 2009

Module 2: Thermodynamics of Irreversible Process and Metabolism (9 hours)

2.1 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.

2.2 Bioenergetics: Standard states in biological systems, biological redox reactions, coupled reactions. ATP and its role in bioenergetics, high energy bond, free energy and entropy change in ATP hydrolysis. Thermodynamic aspects of metabolism, respiration and oxygen storage and transport.

Textbooks

1. P. W. Atkins, J.de Paula, Physical Chemistry: Thermodynamics, Structure, and Change, 10th Edn., Oxford University Press, 2014
2. R. J. Silbey, R. A. Alberty, M. G. Bawendi, Physical Chemistry, 4th Edn., John Wiley & Sons, 2005
3. David L Nelson, Michael M Cox, Lehninger Principles of Biochemistry, 6thEdn., Mc Millan Publishers, 2013

Reference

1. Samuel Glasstone, Thermodynamics for Chemists, Read Books, 2007

Module 3: Statistical Thermodynamics for Material Science (18 hours)

3.1 Types of particles and their arrangements, Sterling's approximation, macrostates and microstates, Boltzmann distribution law, partition function and its physical significance, phase space, different ensembles- canonical, microcanonical, grand canonical; partition function, distinguishable and indistinguishable molecules, relation between partition function and thermodynamic functions(E, S, Cv, P, A), separation of partition function- derivation of translational, rotational, vibrational and electronic partition functions. Thermal de-Broglie wavelength.

3.2 Calculation of thermodynamic functions. Sakur-Tetrode equation for entropy of monoatomic gas, statistical formulation of third law of thermodynamics, thermodynamic probability and entropy, residual entropy, heat capacity of gases - classical and quantum theories, equipartition principle, nuclear spin statistics and heat capacity of hydrogen.

Textbooks

1. M.C. Gupta, Statistical Thermodynamics, 2nd Edn., New Age International, 2007
2. B. K. Agarwal, Statistical Mechanics, 2nd Edn., New Age International, 2013

Reference

1. D. A. McQuarrie, Statistical Mechanics, University Science Books, 2011
2. B. Widom, Statistical Mechanics: A Concise Introduction for Chemists, Cambridge University Press, 2002

3. A. Cooksy, Physical Chemistry: Thermodynamics, Statistical Mechanics, and Kinetics, Pearson Education, 2013
4. Leonard K. Nash, Elements of Statistical Thermodynamics, 2nd Edn., Dover Books, 2006

Module4: Material Properties through Quantum Statistics (9 hours)

4.1 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.

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

4.3 Application in nonequilibrium statistical thermodynamics: chemical kinetics, transport phenomena, real gases (basic idea only).

4.4 Basic theory of computer simulations: Molecular Dynamics, Monte Carlo methods.

Textbooks

1. M. C. Gupta, Statistical Thermodynamics, 2nd Edn., New Age International, 2007
2. B. K. Agarwal, Statistical Mechanics, 2nd Edn., New Age International, 2013

Reference

1. D. A. McQuarrie, Statistical Mechanics, University Science Books, 2011
2. B. Widom, Statistical Mechanics: A Concise Introduction for Chemists, Cambridge University Press, 2002
3. A. Cooksy, Physical Chemistry: Thermodynamics, Statistical Mechanics, and Kinetics, Pearson Education, 2013
4. Leonard K. Nash, Elements of Statistical Thermodynamics, 2nd Edn., Dover Books, 2006

BMCP102: GROUP THEORY AND INTRODUCTORY QUANTUM MECHANICS

Credit: 4 **Total Hours: 72**

Objectives

- To familiarize the theoretical concepts in science.
- To understand the idea about handling many electron systems.
- To understand molecular symmetry, point groups and crystal symmetry
- To understand great orthogonality theorem
- To understand applications of group theory in spectroscopy

Outcome

- Students will be skilled in problem solving, critical thinking and analytical reasoning as applied to scientific problems.
- Able to arrive at Schrodinger wave equation
- Able to solve problems related to many electron systems
- Able to find out the symmetry groups of all molecules
- Able to apply orthogonality theorem to molecules and to construct character table.
- Able to find out the allowed transitions in molecules using character table.

Module 1: Fundamentals of Quantum Mechanics (12 hours)

1.1 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.

Angular Momentum in Quantum Mechanics: Operators for angular momentum, commutation rules, ladder operators, significance. Atomic term symbols, microstates, Spin-orbit coupling, L-S coupling, j-j coupling, selection rules in atomic spectroscopy, Zeeman effect, Spectroscopic term symbols for diatomic molecules.

1.3 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.

Textbooks

1. R. Anantharaman, Fundamentals of Quantum Chemistry, Macmillan India, 2000
2. R.K. Prasad, Quantum Chemistry, 3rdEdn., New Age International, 2006
3. A. K. Chandra, Introduction to Quantum Chemistry, 4th Edn., Tata McGraw Hill, 2006

Reference

1. I.N. Levine, Quantum Chemistry, 6thEdn., Pearson Education Inc., 2009
2. P. W. Atkins, R. S. Friedman, Molecular Quantum Mechanics, 5th Edn., Oxford University Press, 2011
3. D.A. McQuarrie, Quantum Chemistry, University Science Books, 2008
4. J.P. Lowe, K. Peterson, Quantum Chemistry, 3rdEdn., Academic Press, 2006
5. T. Engel, Quantum Chemistry and Spectroscopy, Pearson Education, 2006
6. H. Metiu, Physical Chemistry: Quantum Mechanics, Taylor & Francis, 2006
7. L. Pauling, E.B. Wilson, Introduction to Quantum Mechanics, McGraw Hill, 1935
8. M. S. Pathania, Quantum Chemistry and Spectroscopy (Problems & Solutions), Vishal Publications, 1984

Module 2: Applications of Quantum Mechanics (24hours)

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, Laguerre and Legendre Polynomials (basic 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.

Textbooks

1. R. Anantharaman, Fundamentals of Quantum Chemistry, Macmillan India, 2000
2. R. K. Prasad, Quantum Chemistry, 3rdEdn., New Age International, 2006
3. M. S. Pathania, Quantum Chemistry and Spectroscopy (Problems & Solutions), Vishal Publications, 1984

Reference

1. I. N. Levine, Quantum Chemistry, 6th Edn., Pearson Education Inc., 2009
2. P. W. Atkins, R. S. Friedman, Molecular Quantum Mechanics, 5th Edn., Oxford University Press, 2011
3. D. A. McQuarrie, Quantum Chemistry, University Science Books, 2008
4. J. P. Lowe, K. Peterson, Quantum Chemistry, 3rd Edn., Academic Press, 2006
5. T. Engel, Quantum Chemistry and Spectroscopy, Pearson Education, 2006
6. H. Metiu, Physical Chemistry: Quantum Mechanics, Taylor & Francis, 2006
7. L. Pauling, E. B. Wilson, Introduction to Quantum Mechanics, McGraw Hill, 1935

Module 3: Symmetry and Point Groups (9 hours)

3.1 Symmetry elements, symmetry operations, point groups, classes, abelian and cyclic groups, group multiplication tables-classes in a group and similarity transformation. Symmetry in crystals (basic idea only) -32 crystallographic point groups (no derivation), Hermann-Mauguin symbols. Space groups: Screw axis and Glide plane.

Textbooks

1. K. Veera Reddy, Symmetry and Spectroscopy of Molecules, 2nd Edn., New Age Science Ltd., 2009
2. S. Swarnalakshmi, T. Saroja, R.M. Ezhilarasi, A Simple Approach to Group Theory in Chemistry, Universities Press, 2008

Reference

1. F.A. Cotton, Chemical Applications of Group Theory, 3rdEdn., Wiley Eastern, 2008
2. L. H. Hall, Group Theory and Symmetry in Chemistry, McGraw Hill,1969
3. M.G. Arora, Group Theory in Chemistry and Physics, Anmol Publications Pvt. Ltd., 2002
4. R. Ameta, Symmetry and Group Theory in Chemistry, New Age International Pvt. Ltd., 2012

5. U. C. Agarwala, H. L. Nigam, Sudha Agrawal, S. S. Kalra, Molecular Symmetry in Chemistry via Group Theory, Ane Books Pvt. Ltd., 2016
6. Robert L. Carter, Molecular Symmetry and Group Theory, John Wiley & Sons, 1997
7. Gurdeep Raj, Ajay Kumar Bhagi, Vinod Jain, Group Theory & Symmetry in Chemistry, Krishna Prakashan Media (P) Ltd, 2017
8. Hans H. Jaffe, Milton Orchin, Symmetry in Chemistry, Dover Publications Inc., 2003
9. David M. Bishop, Group Theory and Chemistry, Dover Publications, 1993

Module 4: Group Theory in Molecular Symmetry (18 hours)

4.1 Matrix representation of symmetry operations (C_{2V} and C_{3V} 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_{3v} and C_{4v}. Direct product of representations and its application. Molecular dissymmetry and optical activity.

Textbooks

1. K. Veera Reddy, Symmetry and Spectroscopy of Molecules, 2nd Edn., New Age Science Ltd., 2009
2. S. Swarnalakshmi, T. Saroja, R. M. Ezhilarasi, A Simple Approach to Group Theory in Chemistry, Universities Press, 2008
3. A.S. Kunju, G. Krishnan, Group Theory and its Applications in Chemistry, 2nd Edn., PHI Learning, 2010
4. V. Ramakrishnan, M.S. Gopinathan, Group Theory in Chemistry, 2nd Edn., Vishal Publications, 2013

Reference

1. F. A. Cotton, Chemical Applications of Group Theory, 3rd Edn., Wiley Eastern, 2008
2. L. H. Hall, Group Theory and Symmetry in Chemistry, McGraw Hill,1969
3. M. G. Arora, Group Theory in Chemistry and Physics, Anmol Publications Pvt. Ltd., 2002
4. R. Ameta, Symmetry and Group Theory in Chemistry, New Age International Pvt. Ltd., 2012
5. U. C. Agarwala, H. L. Nigam, Sudha Agrawal, S. S. Kalra, Molecular Symmetry in Chemistry via Group Theory, Ane Books Pvt. Ltd., 2016
6. Robert L Carter, Molecular Symmetry and Group Theory, John Wiley & Sons, 1997

7. Gurdeep Raj, Ajay Kumar Bhagi, Vinod Jain, Group Theory & Symmetry in Chemistry, Krishna Prakashan Media (P) Ltd, 2017
8. Hans H. Jaffe, Milton Orchin, Symmetry in Chemistry, Dover Publications Inc., 2003
9. David M. Bishop, Group Theory and Chemistry, Dover Publications, 1993
10. A. Vincent, Molecular Symmetry and Group Theory: A Programmed Introduction to Chemical Applications, 2nd Edn., Wiley, 2013

Module 5: Application of Group Theory in Spectroscopy (9 hours)

5.1 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_2O, Trans N_2F_2 and NH_3usingCartesian 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.

Textbooks

1. K. Veera Reddy, Symmetry and Spectroscopy of Molecules, 2nd Edn., New Age Science Ltd., 2009
2. S. Swarnalakshmi, T. Saroja, R. M. Ezhilarasi, A Simple Approach to Group Theory in Chemistry, Universities Press, 2008
3. A. S. Kunju, G. Krishnan, Group Theory and its Applications in Chemistry, 2nd Edn., PHI Learning, 2010
4. V. Ramakrishnan, M. S. Gopinathan, Group Theory in Chemistry, 2nd Edn., Vishal Publications, 2013

Reference

1. F. A. Cotton, Chemical Applications of Group Theory, 3rd Edn., Wiley Eastern, 2008
2. L. H. Hall, Group Theory and Symmetry in Chemistry, McGraw Hill,1969
3. M. G. Arora, Group Theory in Chemistry and Physics, Anmol Publications Pvt. Ltd., 2002
4. R. Ameta, Symmetry and Group Theory in Chemistry, New Age International Pvt. Ltd., 2012
5. U. C. Agarwala, H. L. Nigam, Sudha Agrawal, S. S. Kalra, Molecular Symmetry in Chemistry via Group Theory, Ane Books Pvt. Ltd., 2016
6. Robert L Carter, Molecular Symmetry and Group Theory, John Wiley & Sons, 1997

7. Gurdeep Raj, Ajay Kumar Bhagi, Vinod Jain, Group Theory & Symmetry in Chemistry, Krishna Prakashan Media (P) Ltd, 2017
8. Hans H. Jaffe, Milton Orchin, Symmetry in Chemistry, Dover Publications Inc., 2003
9. David M. Bishop, Group Theory and Chemistry, Dover Publications, 1993
10. A. Vincent, Molecular Symmetry and Group Theory: A Programmed Introduction to Chemical Applications, 2nd Edn., Wiley, 2013

BMCP103: CHEMISTRY OF METAL COMPLEXES

Credit: 4 **Total Hours: 72**

Objectives

- To understand structural aspects and bonding in transition metal ligand complexes
- To study in detail electronic spectra and magnetic properties of transition metal ligand complexes.
- To elucidate the structure of metal complexes using electronic spectra and magnetic moments.
- To learn theory of kinetics and mechanism of reactions in metal complexes.
- To understand stereochemistry of coordination compounds.
- To learn the coordination chemistry of inner transition elements.

Outcome

At the successful completion of this course, the student is supposed to acquire thorough knowledge on:

- Various aspects of structure and bonding in transition metal ligand complexes
- Electronic spectra and magnetic properties of transition metal ligand complexes
- Predict the structure from spectral and magnetic data.
- Kinetics and mechanism of reactions in metal complexes
- Stereochemistry of coordination compounds
- Coordination chemistry of inner transition elements.

Module 1: Structural Theories of Metal Ligand Complexes (18 hours)

1.1 Classification of complexes based on coordination numbers and possible geometries. Sigma and pi bonding ligands such as CO, NO, CN-, R_3P, and Ar_3P. HSAB concept, thermodynamic aspects of complex formation, Irving-William order of stability, chelate effect and macrocyclic effect.

1.2 Splitting of d orbitals in octahedral, tetrahedral, square planar, square pyramidal and trigonalbipyramidal fields, LFSE, Dq values, Jahn Teller 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.

Module 2: Properties of Transition Metal Ligand Complexes (18 hours)

2.1 Electronic Spectra of complexes-Term symbols of d^n system, Racah parameters, splitting of terms in weak and strong octahedral and tetrahedral fields. Correlation diagrams for d^n and d^{10-n} 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 crossover, 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.

Textbooks (Modules 1 and 2)

1. J. E. Huheey, E. A. Keiter, R. L. Keiter, O. K. Medhi, Inorganic Chemistry: Principles of Structure and Reactivity, 4thEdn., Pearson Education, 2006
2. R. Sarkar, General and Inorganic Chemistry: Volume II, New Central Book Agency, 2014

Reference (Modules 1 and 2)

1. N. N. Greenwood, A. Earnshaw, Chemistry of the Elements, 2nd Edn., Butterworth Heinemann, 2004
2. J. D. Lee, Concise Inorganic Chemistry, 5th Edn., Wiley India (P) Ltd., 2010
3. K. F. Purcell, J. C. Kotz, Inorganic Chemistry, Holt-Saunders, 1977
4. B. E. Douglas, D. H. McDaniel, J. J. Alexander, Concepts and Models of Inorganic Chemistry, 3rdEdn., Wiley-India, 2007
5. P. Atkins, T. Overton, J. Rourke, M. Weller, F. Armstrong, Inorganic Chemistry, 5thEdn., Oxford University Press, 2010

Module 3: Stereochemistry of Octahedral and Tetrahedral Complexes (9 hours)

3.1 Geometrical and optical isomerism in octahedral and tetrahedral 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 catalysed by coordination compounds.

3.2 Linkage isomerism-electronic and steric factors affecting linkage isomerism. Symbiosis-hard and soft ligands, Prussian blue and related structures.

Textbooks

1. J. E. Huheey, E. A. Keiter, R. L. Keiter, O. K. Medhi, Inorganic Chemistry: Principles of Structure and Reactivity, 4th Edn., Pearson Education, 2006
2. B. E. Douglas, D. H. McDaniel, J. J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Edn., Wiley-India, 2007

Reference

1. K. F. Purcell, J. C. Kotz, Inorganic Chemistry, Holt-Saunders, 1977
2. P. Atkins, T. Overton, J. Rourke, M. Weller, F. Armstrong, Inorganic Chemistry, 5th Edn., Oxford University Press, 2010

Module 4: Chemistry of Rare Earth Elements (9 hours)

4.1 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.

4.2 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.

Textbooks

1. J. E. Huheey, E. A. Keiter, R. L. Keiter, O. K. Medhi, Inorganic Chemistry: Principles of Structure and Reactivity, 4th Edn., Pearson Education, 2006
2. R. Sarkar, General and Inorganic Chemistry: Volume II, New Central Book Agency, 2014

Reference

1. N. N. Greenwood, A. Earnshaw, Chemistry of the Elements, 2nd Edn., Butterworth Heinemann, 2004
2. J. D. Lee, Concise Inorganic Chemistry, 5th Edn., Wiley India (P) Ltd., 2010
3. K. F. Purcell, J. C. Kotz, Inorganic Chemistry, Holt-Saunders, 1977
4. B. E. Douglas, D. H. McDaniel, J. J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Edn., Wiley-India, 2007

5. P. Atkins, T. Overton, J. Rourke, M. Weller, F. Armstrong, Inorganic Chemistry, 5th Edn., Oxford University Press, 2010

Module 5: Transition Metal Complexes and Their Reactions (18 hours)

5.1 Stability of complexes, stepwise and overall formation constants, nucleophilic substitution reactions in square planar complexes – mechanism and kinetics, theory and applications of trans effect, trans influence.

5.2 Kinetics and mechanism of octahedral substitution- water exchange, dissociative and associative mechanisms, racemization reactions, solvolytic reactions (acidic and basic).

5.3 Oxidation reduction reactions: inner sphere and outer sphere reactions and mechanisms, excited electron transfer reactions

Textbooks

1. B. E. Douglas, D. H. McDaniel, J. J. Alexander, Concepts and Models of Inorganic Chemistry, 3rdEdn., Wiley-India, 2007.
2. J. E. Huheey, E. A. Keiter, R. L. Keiter, O. K. Medhi, Inorganic Chemistry: Principles of Structure and Reactivity, 4thEdn., Pearson Education, 2006
3. B. R. Puri, L. R. Sharma, M. S. Pathania, Principles of Physical Chemistry,47th Edn., Vishal Publishing Co., 2018

Reference

1. K. F. Purcell, J. C. Kotz, Inorganic Chemistry, Holt-Saunders, 1977
2. F. Basolo, R.G. Pearson, Mechanisms of Inorganic Reaction, John Wiley & Sons, 2006
3. F. A. Cotton, G. Wilkinson, C. A. Murillo, M. Bochmann, Advanced Inorganic Chemistry, 6thEdn., John Wiley & Sons Inc., 1999
4. R. G. Wilkins, Kinetics and Mechanism of Reactions of Transition Metal Complexes, Wiley-VCH Verlag GmbH & Co., 2002
5. R. W. Hay, Reaction Mechanisms of Metal Complexes, Horwood Publishing Ltd., 2000

BMCP104: BASIC ORGANIC CHEMISTRY FOR POLYMER CHEMISTS

Credit: 4 **Total Hours: 72**

Objectives

- To understand the various electronic factors deciding the molecular properties
- To study in detail how to propose mechanism for simple organic reactions
- To recognize and distinguish between aromatic and antiaromatic compounds by their structures.
- To know the properties of aromatic and antiaromatic compounds, and the chemical consequences of aromaticity.
- To gain a thorough knowledge of symmetry properties of organic molecules.
- Differentiate chiral and achiral molecules.
- To learn various conformations of cyclic and acyclic compounds

Outcome

At the successful completion of this course, the student is supposed to acquire thorough knowledge on:

- The common reactions undergone by organic compounds and the method to propose a suitable mechanism for it
- Analyse aromaticity of a compound and follow the various reactions shown by aromatic compounds
- Recognize and draw structural isomers (constitutional isomers), stereoisomers including enantiomers and diastereomers, racemic mixture, and meso compounds.
- Identify the stereocenters in a molecule and assign the configuration as R or S.

Module 1: Reaction Mechanisms (18 hours)

1.1 IUPAC nomenclature of spiro, bicyclic, heterocyclic compounds, designation of organic reactions.

1.2 Electronic Effects and their applications: inductive effect, electromeric effect, resonance effect, hyperconjugation, steric effect- steric acceleration and steric retardation, Super acids and bases, proton sponges, B strain and F strain. Bonding weaker than covalent bonds- Hydrogen bonding and its effect of physical and chemical properties, Directional nature of hydrogen bond. Carbon bonds, trexal and tetral bonds (introduction)

1.3 Aliphatic Substitution reactions: IUPAC Classification and Nomenclature of reaction mechanisms. Review of nucleophilic and electrophilic substitution at aliphatic carbon (S_N1, S_N2, S_N1', S_N2', S_Ni, SET, $S_{RN}1$ S_E1, S_E2), effect of substrate, reagent, leaving group and solvent. Neighbouring group participation- evidence, participation of O, S, X, phenonium, sigma and pi bonds Mixed S_N1 and S_N2.

1.4 Elimination reactions- Elimination (E_1, E_2 & E_1CB). Orientation of the double bond: Zaitsev Elimination and Hofmann Elimination, Bredt's Rule. Anti elimination and Syn elimination. Mechanism and orientation in Hofmann degradation, Pyrolytic eliminations and Corey-Winter reaction. Elimination vs. substitution.

1.5 Addition reactions (regioselectivity: Markovnikov's addition carbocation mechanism, anti-Markovnikov's addition-radical mechanism. Oxymercuration- demercuration, halolactonisation, hydroboration – oxidation.

Textbooks

1. M. B. Smith, J. March, March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure, 6th Edn., Wiley, 2006
2. J. Clayden, N. Greeves, S. Warren, Organic Chemistry, 2ndEdn. Oxford University Press, 2012

Reference

1. R. Bruckner, Advanced Organic Chemistry: Reaction Mechanisms, Academic Press, 2002
2. M. B. Smith, March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure, 7th Edn., Wiley, 2015
3. F. A. Carey, R. J. Sundberg, Advanced Organic Chemistry, Part A: Structure and Mechanisms, 5th Edn., Springer, 2007
4. T.H. Lowry, K.S. Richardson, Mechanism and Theory in Organic Chemistry, 2nd Edn., Harper & Row, 1981
5. T. Ishikawa (Ed.), Super Bases for Organic Synthesis, Wiley, 2008
6. J. M. Coxon, R.O.C. Norman, Principles of Organic Synthesis, 2nd Edn., Springer, 2012
7. J. P. Trivedi, Reaction Intermediates in Organic Chemistry, University Granth Nirman Board, Ahmedabad
8. Peter Sykes, A Guidebook to Mechanism in Organic Chemistry, 6thEdn., Orient Longman Ltd., 1997

9. T. Okuyama, H. Maskill, Organic Chemistry: A Mechanistic Approach, Oxford University Press, 2014

Module 2: Aromaticity and Reaction Mechanisms (18 hours)

2.1 Huckel's rule. Criteria for aromaticity and anti-aromaticity- structural, electronic and magnetic criteria. Homo-aromaticity, NMR as a tool for aromaticity, Diamagnetic and paramagnetic anisotropy.

2.2 Examples of neutral and charged aromatic systems, Huckel Molecular Orbital Theory (qualitative idea only- derivations not expected) of cyclopropenyl, cyclobutenyl, cyclopentenyl systems and benzene tropylium cation. Frost Circle representation. Annulenes-detailed study. Harmonic oscillator model of aromaticity (HOMA) - elementary idea only. Nucleus-independent chemical shift (NICS)-elementary idea only.

2.4 Aromaticity in fused rings: aromaticity of azulenes, pentalene, heptalene, tropones, tropolones, hetrocyclics, fullerenes, triafulvene, pentafulvene,heptafulvene, triafulvalene, pentafulvalene, heptafulvalene, chrysene, pyrene and coronene etc.

2.5 Electrophilic Aromatic Substitution: Arenium ion mechanism, orientation and reactivity in monosubstituted benzene rings, ortho/para ratio, ipso attack.

2.6 Nucleophilic Aromatic substitution: S_N1, S_NAr, SR_N1 and benzyne mechanisms, reactivity - effect of substrate structure, leaving group, and attacking nucleophile.

2.7 Organic reactions involving benzene diazonium salts- Meerwin reaction, Gomberg reaction, Pschorr reaction, Chloromethylation of aromatic systems- Gatterman's formylation, Gatterman-Koch formylation, Hoesch acylation, Vilsmeyer formylation. Von Richter rearrangement.

Textbooks

1. J. Clayden, N. Greeves, S. Warren, Organic Chemistry, 2nd Edn. Oxford University Press, 2012
2. F. A. Carey, R. J. Sundberg, Advanced Organic Chemistry, Part A and B, 5th Edn., Springer, 2009.
3. M. B. Smith, March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure, 7th Edn., Wiley, 2015

Reference

1. Peter Sykes, A Guidebook to Mechanism in Organic Chemistry, 6th Edn., Orient Longman Ltd., 1997
2. P. S. Kalsi, Organic Reactions and Their Mechanisms, New Age Science Ltd., 2017

Module 3: Stereochemistry of Carbon Compounds (18 hours)

3.1 Criteria for optical activity/chirality, Symmetry operations and elements of symmetry (Axis, plane, centre, alternating axis of symmetry with suitable examples), molecules with one or more than one centre of chirality (qualitative idea only), Molecules with C, N and S based chiral centres (qualitative idea only).

3.2 Projection formulae: -Fischer, Newman, Sawhorse and Flying Wedge projections, interconversion of various projection formulae with suitable examples.

3.3 Notation of configuration of optical isomers: - Absolute configuration and R/S nomenclature, relative configuration and D/L configuration, Erythro-threo nomenclature, enantiomers, racemic modifications, meso compounds and diastereoisomers, constitutionally symmetrical and unsymmetrical chiral molecules (qualitative idea only), configuration and conformational stereoisomers (elementary ideas only).

3.4 Resolution and methods of resolution: Mechanical/physical separation, biochemical separation, chemical method and chromatographic separation; optical purity and enantiomeric excess (chromatographic, enzymatic and NMR method).

3.5 Axial, planar and helical chirality: Principles of axial/planar chirality, stereochemistry and absolute configuration of allenes, spiranes, biphenyls derivatives (atropisomerism) and binaphthyls; stereochemistry of molecules with planar chirality - ansa compounds and cyclophanes; stereochemistry of molecules with helical chirality.

3.6 Topicity of ligands and faces: Homotopic ligands/atoms/groups/faces with examples, enantiotopic ligands/atoms/groups/faces with examples and diastereotopic ligands/atoms/groups/faces with examples; Symmetry/Substitution-Addition criteria for topicity; Nomenclature of stereoheterotopic ligands/faces (pro-R/pro-S and Re/Si); NMR distinction of enantiotopic/diastereotopic ligands.

3.7 Prostereoisomerism and stereoisomerism-chemical and biochemical transformation of heterotopic ligands and faces.

Textbooks

1. P. S. Kalsi, R. S. Oza, Organic Reactions Stereochemistry and Mechanism - Through Solved Problems, New Age International (P) Ltd., 2018
2. D. Nasipuri, Stereochemistry of Organic Compounds: Principles and Applications, 4thEdn., New Academic Science Ltd., 2012

Reference

1. J. Clayden, N. Greeves, S. Warren, Organic Chemistry, 2nd Edn. Oxford University Press, 2012

2. J. M. Coxon, R. O. C. Norman, Principles of Organic Synthesis, 2nd Edn., Springer, 2012
3. Peter Sykes, A Guidebook to Mechanism in Organic Chemistry, 6th Edn., Orient Longman Ltd., 1997
4. D. G. Morris, Stereochemistry, RSC Tutorial Chemistry Text 1, 2001
5. E. L. Eliel, S. H. Wilen, Stereochemistry of Organic Compounds, John Wiley & Sons, 1994

Module 4: Conformation Analysis of Acyclic and Cyclic Organic Compounds(18 hours)

4.1 Conformational analysis of common acyclic systems-ethane, substituted ethanes, propane, *n*-butane, *n*-pentane, acetaldehyde, propionaldehyde and acetone. Factors affecting conformational stability of these molecules.

4.2 Conformational analysis of cyclic systems: Conformations of carbocyclic rings from three to eight. Conformations of substituted cyclohexanes, cyclohexene, cyclohexanone, 2-halocyclohexanones and alkylidenecyclohexanes. Conformational structures of heterocycles-anomeric effects in hexoses, piperidine and N-methylpiperidine. Fused and bridged bicyclic systems-decalin, adamantane, congressane, and norborane. 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 eliminations, nucleophilic substitution reactions, formation and cleavage of epoxides, esterification and hydrolysis, hydride reduction of cyclohexanones and oxidation of cyclohexanols to cyclohexanone by chromic acid. Effect of conformation on elimination reactions acyclic systems.

Textbooks

1. D. Nasipuri, Stereochemistry of Organic Compounds: Principles and Applications, 4th Edn., New Academic Science Ltd., 2012
2. P. S. Kalsi, Stereochemistry Conformation and Mechanism, 8thEdn., New Age International (P) Ltd., New Delhi, 2015

Reference

1. E. L. Eliel, S. H. Wilen, Stereochemistry of Organic Compounds, John Wiley & Sons, 1994
2. D. G. Morris, Stereochemistry, 1stEdn., RSC Tutorial Chemistry Text 1, 2001

3. T. Okuyama, H. Maskill, Organic Chemistry: A Mechanistic Approach, Oxford University Press, 2014

SEMESTER II

BMCP205: ADVANCED TOPICS IN THEORETICAL CHEMISTRY

Credit: 3 **Total Hours: 54**

Objectives

- To familiarize the theoretical concepts of many electron systems.
- To understand the importance of approximation methods in theoretical Chemistry
- To familiarize the chemical aspects of boning
- To get introduced to computational chemistry

Outcome

- Knowledge of higher level theoretical concepts
- Ability to understand molecular reactivity based on chemical bonding
- Able to solve problems related to many electron systems
- Work with computational softwares

Module 1: Hydrogen Atom (9 hours)

1.1 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.

Textbooks

1. R. Anantharaman, Fundamentals of Quantum Chemistry, Macmillan India, 2000
2. R. K. Prasad, Quantum Chemistry, 3rdEdn., New Age International, 20066

Reference

1. I. N. Levine, Quantum Chemistry, 6th Edn., Pearson Education Inc., 2009
2. P.W. Atkins, R.S. Friedman, Molecular Quantum Mechanics, 5thEdn., Oxford University Press, 2011
3. D. A. McQuarrie, Quantum Chemistry, University Science Books, 2008
4. J. P. Lowe, K. Peterson, Quantum Chemistry, 3rd Edn., Academic Press, 2006
5. T. Engel, Quantum Chemistry and Spectroscopy, Pearson Education, 2006

6. H. Metiu, Physical Chemistry: Quantum Mechanics, Taylor & Francis, 2006

Module 2: Approximation Methods (18 hours)

2.1 Independent Particle Model: Example of Helium atom, Electron correlation problem, Calculation of ground state energy, Comparison with experimental value.

2.2 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.

2.3 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 1D box with slanted bottom, anharmonic oscillator

2.4 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.

Textbooks

1. R. Anantharaman, Fundamentals of Quantum Chemistry, Macmillan India, 2000
2. R. K. Prasad, Quantum Chemistry, 3rdEdn., New Age International, 2006

Reference

1. I. N. Levine, Quantum Chemistry, 6th Edn., Pearson Education Inc., 2009
2. P. W. Atkins, R. S. Friedman, Molecular Quantum Mechanics, 5th Edn., Oxford University Press, 2011
3. D. A. McQuarrie, Quantum Chemistry, University Science Books, 2008
4. J. P. Lowe, K. Peterson, Quantum Chemistry, 3rd Edn., Academic Press, 2006
5. T. Engel, Quantum Chemistry and Spectroscopy, Pearson Education, 2006
6. H. Metiu, Physical Chemistry: Quantum Mechanics, Taylor & Francis, 2006

Module 3: Chemical Bonding and Hybridisation (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. Huckel 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.

Textbooks

1. R. Anantharaman, Fundamentals of Quantum Chemistry, Macmillan India, 2000
2. R. K. Prasad, Quantum Chemistry, 3rdEdn., New Age International, 2006

Reference

1. I. N. Levine, Quantum Chemistry, 6th Edn., Pearson Education Inc., 2009
2. P. W. Atkins, R. S. Friedman, Molecular Quantum Mechanics, 5th Edn., Oxford University Press, 2011
3. D. A. McQuarrie, Quantum Chemistry, University Science Books, 2008
4. J. P. Lowe, K. Peterson, Quantum Chemistry, 3rd Edn., Academic Press, 2006
5. T. Engel, Quantum Chemistry and Spectroscopy, Pearson Education, 2006

Module 5: Computational Aspects in Chemistry (9 hours)

5.1 Introduction: Fields of application; Potential Energy Surfaces: Stationary points, saddle point, local and global minima, their significance.

5.2 Molecular Mechanics: Concept of Force Field, its components for bond stretching, bending, torsional motion, non-bonded and electrostatic interactions. Examples for force fields: MM, AMBER and CHARMM.

5.3 Molecular Dynamics: General Principles of MD simulations, Design constraints: Microcanonical, Canonical, isothermal-isobaric, generalized ensembles; Applications and limitations of MD.

Textbooks

1. J.H.Jensen, E.G. Lewars, Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics, 2nd Edn., Springer, 2011
2. F. Jensen, Introduction to Computational Chemistry, 2nd Edn., John Wiley & Sons, 2007
3. A. R. Leach, Molecular Modelling: Principles and Applications, 2nd Edn., Pearson Education Ltd., 2001

Reference

1. J.P. Fackler Jr., L.R. Falvello (Eds.), Techniques in Inorganic Chemistry: Chapter 4, CRC Press, 2011
2. K.I. Ramachandran, G. Deepa, K. Namboori, Computational Chemistry and Molecular Modeling: Principles and Applications, Springer, 2008
3. A. Hinchliffe, Molecular Modelling for Beginners, 2nd Edn., John Wiley & Sons, 2008
4. C.J. Cramer, Essentials of Computational Chemistry: Theories and Models, 2nd Edn., John Wiley & Sons, 2004
5. D.C. Young, Computational Chemistry: A Practical Guide for Applying Techniques Real-World Problems, John Wiley & Sons, 2001

BMCP206: PRINCIPLES OF MOLECULAR SPECTROSCOPY AND SOLID STATE

Credit: 4 **Total Hours: 72**

Objectives

The objective of this course is to make the student aware of /enable to

- Study the kinetics and dynamics of various reactions
- The theory of interaction of light and matter
- Understand various energy levels of molecules/particles
- Elucidate the structure from spectral data
- The basic instrumentation of various spectroscopic methods

Outcome

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

- To determine the rate of reaction using different methods
- Understand the interaction of various components of EM radiation with matter
- Calculate the energy levels, interuclear distance etc.
- To predict the structure/spectrum of molecules

Module 1: Spectroscopic Techniques for Material Science (27 hours)

1.1 Origin of spectra: origin of different spectra and the regions of the electromagnetic spectrum, factors affecting spectral line width and intensity, signal to noise ratio, Born Oppenheimer approximation, importance of molecular spectroscopy.

1.2 Microwave spectroscopy: classification of molecules, interaction of radiation, rotational spectra of rigid diatomic molecules, selection rules, calculation of intermolecular distance, intensity of rotational lines, relative population of energy levels, derivation of J_{max}, effect of isotopic substitution, 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: Vibrating diatomic molecule, harmonic oscillator, anharmonicity, 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 of carbon dioxide and water, combination and difference bands, Fermi resonance, finger print region and group vibrations, effect of H-bonding on group frequency, introduction to FTIR and ATR, sampling, applications.

1.4 Raman spectroscopy: scattering of light, polarizability, classical theory and quantum theory of Raman scattering, 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, applications in solid state chemistry.

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, progressions and sequences, Franck-Condon principle, Fortrat parabola, dissociation, predissociation, calculation of heat of dissociation, Birge and Sponer method, photoelectron spectroscopy, elementary idea on lasers.

Textbooks

1. N. Banwell, E.M. McCash, Fundamentals of Molecular Spectroscopy, 5thEdn., Tata McGraw Hill, 2017
2. G. Aruldhas, Molecular Structure and Spectroscopy, Prentice Hall of India, 2008
3. P.S.Sindhu, Fundamentals of Molecular Spectroscopy, New Age International, 2011

Reference

1. R.S. Drago, Physical Methods in Chemistry, Saunders College, 1992
2. H. Gunther, NMR Spectroscopy, Wiley, 1995
3. Atta-ur-Rahman, Nuclear Magnetic Resonance: Basic Principles, Springer, 2008
4. D.N. Sathyanarayan, Handbook of Molecular Spectroscopy, IK International Publishing, 2015
5. H.S. Randhawa, Modern Molecular Spectroscopy, Macmillan India Ltd., 2009

Module 2: Resonance Techniques for the Characterisation of Materials (27 hours)

2.1 NMR spectroscopy: spin, nuclear energy levels, population of energy levels, resonance condition, Larmor precession, chemical shift, spin – spin coupling, representation of proton nmr spectrum, spin systems - examples, exchange phenomenon, factors influencing coupling, Karplus relationship.

2.2 FTNMR, FID, relaxation methods and their determination, second order effects on spectra, simplification of second order spectra - chemical shift reagents, high field NMR, double resonance, off resonance decoupling, NOE effect, two dimensional NMR, COSY and HETCOR, ^{13}C NMR, ^{13}C chemical shift and structure correlation, introduction to solid state NMR, MAS.

2.3 EPR spectroscopy: principle, representation of spectrum, spectrum of methyl radical, g factor, factors affecting g values, fine structure and hyperfine structure, zero field splitting and Kramers' degeneracy, McConnell equation, applications.

2.4 An elementary study of NQR spectroscopy: energy levels, effect on NMR spectrum, applications.

2.5 Mossbauer spectroscopy: principle, Doppler effect, recording of spectrum, chemical shift, factors determining chemical shift, quadrupole interaction, magnetic hyperfine interaction, applications, spectrum of simple molecules.

Textbooks

1. N. Banwell, E.M. McCash, Fundamentals of Molecular Spectroscopy,5thEdn., Tata McGraw Hill, 2017
2. G. Aruldhas, Molecular Structure and Spectroscopy, Prentice Hall of India, 2008
3. P. S. Sindhu, Fundamentals of Molecular Spectroscopy, New Age International, 2011

Reference

1. R. S. Drago, Physical Methods in Chemistry, Saunders College, 1992
2. H. Gunther, NMR Spectroscopy, Wiley, 1995
3. Atta-ur-Rahman, Nuclear Magnetic Resonance: Basic Principles, Springer, 2008
4. D. N. Sathyanarayan, Handbook of Molecular Spectroscopy, IK International Publishing, 2015
5. H. S. Randhawa, Modern Molecular Spectroscopy, Macmillan India Ltd., 2009

Module 3: Solid State (18 hours)

3.1 Miller Indices, spacing between the planes of a crystal, XRD methods- Bragg's Equation, rotating crystal powder XRD methods, XRD patterns of cubic system and tungsten crystal, determination of structure of sodium chloride by powder method, comparison of the structures of NaCl and KCl.

3.2 Structure factor: atomic scattering factor, coordinate expression for structure factor, structure by Fourier synthesis. Introduction to electron and neutron diffraction studies of crystals.

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

Textbooks

1. Carmelo Giacovazzo, Fundamentals of Crystallography, 3rd Edn., Oxford Science Publications, 2002

2. Peter J. Collings, Michael Hird, Introduction to Liquid Crystals: Chemistry and Physics, 1st Edn., Taylor & Francis, 1997

Reference

1. Donald E. Sands, Introduction to Crystallography, Dover Publications, 1994
2. B. R. Puri, L. R. Sharma, M. S. Pathania, Principles of Physical Chemistry, 47th Edn., Vishal Publishing Co., 2018
3. P.J. Wojtowicz, Ping Sheng, E.B. Priestley, Introduction to Liquid Crystals, Springer, 1974

BMCP207: BIOINORGANIC CHEMISTRY, NUCLEAR CHEMISTRY AND ORGANOMETALLIC COMPOUNDS

Credit: 4 **Total Hours: 72**

Objectives

- To study in detail the methods of synthesis, structure and bonding of various organometallic species
- To generate awareness about the modes of reactions in organometallic compounds
- To give an introduction to the application of organometallic compounds in catalytic pathways used in Industries
- To study in detail the functioning of metals in biological systems
- To learn the chemistry of nuclei and the analytical applications of radionuclides in various fields

Outcome

At the successful completion of this course, the student is supposed to acquire thorough knowledge on:

- various aspects of synthesis, structure and bonding of organometallic compounds
- reactions of organometallic compounds in detail
- mode of homogeneous and heterogeneous organometallic catalysis
- metals in biological systems and metal management in living systems
- applications of radio isotopes in industry and medicine

Module 1: Chemistry of Living Things (18 hours)

1.1 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.

1.2 Chemical Toxicology: Biochemical effects of the metals: Arsenic, Cadmium, Lead and Mercury.

1.3 Chemistry of Photosynthesis: Light reactions: Reaction centre, photosystem, Z-Scheme, Photosystem I and II, structure and function of Mn cluster.

1.4 Metal Management in Living Systems: Iron Storage: Ferritin, Haemosiderin; Iron Transport: Transferrins, Siderophores and their iron transfer mechanisms.

Dioxygen Management: Myoglobin and Haemoglobin, structure, chemistry of oxygen binding, electronic structural changes, functions of Myoglobin and Haemoglobin, Cooperativity of Haemoglobin. Bohr Effect, Picket Fence Model. Haemerythrin and

haemocyanin: structure and mechanism of dioxygen transport.Other storage and transport systems: Metallothioneins, Phytochelatins, Ceruloplasmin and Vanadocytes.

1.5 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.

1.6 Nitrogen Fixation: Diazotrophs, Symbiosis, Nitrogenases and their components, Chemistry of biological nitrogen fixation.

1.7 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, Ribonucleotide reductase, Coenzyme forms of vitamin B12: structures and functions.

1.8 Metals in Medicine: Metals as radiation sources: radionuclides, 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.

Textbooks

1. D.E. Fenton, Biocordination Chemistry, Oxford Science Publication, 1995
2. T. Overton, J. Rourke, F. Armstrong, P. Atkins, M. Weller, Inorganic Chemistry, 5thEdn., Oxford University Press, 2010

Reference

1. J. E. Huheey, E. A. Keiter, R. L. Keiter, O. K. Medhi, Inorganic Chemistry: Principles of Structure and Reactivity, 4thEdn., Pearson Education, 2006
2. F. A. Cotton, G. Wilkinson, C. A. Murillo, M. Bochmann, Advanced Inorganic Chemistry, 6th Edn., John Wiley & Sons Inc., 1999
3. K. F. Purcell, J. C. Kotz, Inorganic Chemistry, Holt-Saunders, 1977
4. B. E. Douglas, D. H. McDaniel, J. J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Edn., Wiley-India, 2007
5. R.W. Hay, Bio Inorganic Chemistry, Ellis Horwood, 1984
6. J. D. Lee, Concise Inorganic Chemistry, 5th Edn., Wiley India (P) Ltd., 2010

Module 2: Applications of Nuclear Chemistry (18hours)

2.1 Radioactive equilibrium: Transient and secular equilibria. Q value, reaction cross sections, threshold energy. Nuclear structure, mass and charge. Nuclear models – shell, liquid

drop, Fermi gas, collective and optical models. Nuclear moments, nuclear forces, binding energy. Semi-empirical mass equation. Stability rules, Magic numbers

2.2 Fission products and fission yield. Neutron capture cross section and critical size. Nuclear energy source – nuclear chain reactions, principles of nuclear reactors. Nuclear fusion reactions and their applications. Principles of counting technique such as GM counter, proportional, ionization and scintillation counters. Cloud chamber. Measurement of radiation doses.

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

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

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

Textbooks

1. H. J. Arnikar, Essentials of Nuclear Chemistry, 4thEdn., New Age International (P) Ltd., 2007
2. U. N.Dash, Nuclear Chemistry, 2ndEdn., S Chand & Sons, 2005
3. J. D. Lee, Concise Inorganic Chemistry, 5th Edn., Wiley India (P) Ltd., 2010

Reference

1. W. D. Loveland, D. J. Morrissey, G. T. Seaborg, Modern Nuclear Chemistry, 1stEdn., John Wiley & Sons, 2006
2. G. Friedlander, J. W. Kennedy, E. S. Macias, J. M. Miller, Nuclear and Radiochemistry, 3rdEdn., John Wiley & Sons, New York, 1981

Module 3: Preparation, Structure and Bonding in Organometallic Compounds

(18 hours)

3.1 Organometallic compounds with linear pi donor ligands-olefins, acetylenes, dienes and allyl complexes-synthesis, structure and bonding.

3.2 Complexes with cyclic pi donors-metallocenes and cyclic arene complexes-structure and bonding. Hapto nomenclature. Carbene and carbyne complexes.

3.3 Preparation, properties, structure and bonding of simple mono and binuclear metalcarbonyls, vibrational spectra of metal carbonyls, metal nitrosyls, metal cyanides and dinitrogen complexes. Polynuclear metal carbonyls with and without bridging.

3.4 Valence electron count (16/18 electron rules). Carbonyl clusters-LNCCS and HNCCS, Isoelectronic and isolobal analogy, Wade-Mingos rules, cluster valence electrons.

Textbooks

1. J. E. Huheey, E. A. Keiter, R. L. Keiter, O. K. Medhi, Inorganic Chemistry: Principles of Structure and Reactivity, 4th Edn., Pearson Education, 2006
2. B.D. Guptha, A.J. Elias, Basic Organometallic Chemistry, Universities Press, 2010

Reference

1. G. L. Miessler, P. J. Fischer, D. A. Tarr, Inorganic Chemistry, 5thEdn., Pearson, 2011
2. N. N. Greenwood, A. Earnshaw, Heinemann, 2004Chemistry of the Elements, 2nd Edn., Butterworth
3. B. E. Douglas, D. H. McDaniel, J. J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Edn., Wiley-India, 2007
4. P. Atkins, T. Overton, J. Rourke, M. Weller, F. Armstrong, Inorganic Chemistry, 5th Edn., Oxford University Press, 2010

Module 4: Chemistry of Organometallic Compounds (9 hours)

4.1 Substitution reactions-nucleophilic ligand substitution, nucleophilic and electrophilic attack on coordinated ligands.

4.2 Addition and elimination reactions-1,2 additions to double bonds, carbonylation and decarbonylation, oxidative addition and reductive elimination, insertion(migration) and elimination reactions.

4.3 Rearrangement reactions, redistribution reactions, fluxional isomerism.

Textbooks

1. J. E. Huheey, E. A. Keiter, R. L. Keiter, O. K. Medhi, Inorganic Chemistry: Principles of Structure and Reactivity, 4th Edn., Pearson Education, 2006
2. P. Atkins, T. Overton, J. Rourke, M. Weller, F. Armstrong, Inorganic Chemistry, 5th Edn., Oxford University Press, 2010

Reference

1. J. D. Lee, Concise Inorganic Chemistry, 5th Edn., Wiley India (P) Ltd., 2010
2. F. A. Cotton, G. Wilkinson, C. A. Murillo, M. Bochmann, Advanced Inorganic Chemistry, 6th Edn., John Wiley & Sons Inc., 1999

3. P. Powell, Principles of Organometallic Chemistry, 2nd Edn., Chapman and Hall, London, 2011.

Module 5: Industrial Applications of Organometallic Compounds (9 hours)

5.1 Homogeneous and heterogeneous organometallic catalysis-alkene hydrogenation using Wilkinson catalyst, Tolman catalytic loops.

5.2 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.

5.3 Carbonylation reactions-Monsanto acetic acid process, carbonylation of butadiene using $Co_2(CO)_8$ catalyst in adipic ester synthesis. Olefin methathesis-synthesis gas based reactions, photodehydrogenation catalyst ("platinum pop"). Palladium catalysed oxidation of ethylene-the Wacker process.

Textbooks

1. J. E. Huheey, E. A. Keiter, R. L. Keiter, O. K. Medhi, Inorganic Chemistry: Principles of Structure and Reactivity, 4th Edn., Pearson Education, 2006
2. P. Atkins, T. Overton, J. Rourke, M. Weller, F. Armstrong, Inorganic Chemistry, 5th Edn., Oxford University Press, 2010

Reference

1. J. D. Lee, Concise Inorganic Chemistry, 5th Edn., Wiley India (P) Ltd., 2010
2. F. A. Cotton, G. Wilkinson, C. A. Murillo, M. Bochmann, Advanced Inorganic Chemistry, 6th Edn., John Wiley & Sons Inc., 1999
3. P. Powell, Principles of Organometallic Chemistry, 2ndEdn., Chapman and Hall, London, 2011

BMCP208: PHYSICAL ORGANIC CHEMISTRY AND ORGANIC REACTIONS

Credit: 4 **Total Hours: 72**

Objectives

- Explain the physical forces controlling a reaction
- With the help of quantum mechanics, students get a clear picture of HOMO –LUMO concepts for the analysis of synchronous reactions
- It intends to enhance a detailed understanding of the concept of the processes of pericyclic reactions and the stereochemical outcomes of these highly stereospecific reaction.
- Study the structure, properties and reactions of various intermediates.

Outcome

- After the course, students can understand various physical and chemical factors controlling organic reactions.
- This module enables the students to understand the underlying mechanism for all photochemical processes.
- The students can understand the importance of intermediate chemistry

Module 1: Basic Concepts in the Determination of Organic Reaction Mechanisms

(18 hours)

1.1 Potential energy vs reaction co-ordinate curve, conceptual idea of Marcus theory, Hammond postulate, reactivity vs. selectivity principle, Curtin-Hammett principle, principle of microscopic reversibility, kinetic versus thermodynamic control of product formation.

1.2 Methods of determining reaction mechanisms- product analysis – determination of the presence of intermediate, isolation, detection and trapping – cross over experiments – isotopic labelling – kinetic isotopic effect – stereo chemical evidence – and kinetic evidence.

1.3 Quantitative treatment of structure on reactivity: Linear free energy relationship (LFER) in determination of organic reaction mechanism, The Hammett equation and its applications, The Taft model, Grunwald-Winstein plots.

1.4 Catalysis: General principles of catalysis, specific and general catalysis, nucleophilic catalysis and covalent catalysis. Phase transfer catalysis and applications. Concept of hard and soft acids and bases- HSAB theory.

Textbooks

1. E. V. Anslyn, D. A. Dougherty, Modern Physical Chemistry, University Science Books, 2005

Reference

1. N. S. Isaacs, Physical Organic Chemistry, 2nd Edn., ELBS/Longman, 1995
2. F. A. Carey, R. J. Sundberg, Advanced Organic Chemistry, Part A: Structure and Mechanisms, 5th Edn., Springer, 2007
3. J. Clayden, N. Greeves, S. Warren, Organic Chemistry, 2nd Edn. Oxford University Press, 2012
4. M. B. Smith, March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure, 7th Edn., Wiley, 2015

Module 2: Concerted Reactions and Their Mechanisms (18 hours)

2.1 Pericyclic Reactions: Classification, electrocyclic, sigmatropic, cycloaddition, chelotropic and ene reactions, Woodward Hoffmann rules, Orbital symmetry correlation approach (i) for the analysis of [2+2] cycloaddition under thermal and photochemical conditions, (ii) for the analysis of Electro cyclic reactions involving 4pi electrons and 6pi electrons under thermal and photochemical conditions.

2.2 FMO analysis of Diels-Alder reaction (stereospecificity, endoselectivity and regioselectivity), synthetic application of Diels-Alder like aldrin and dieldrin, Ene reactions (with HOMO-LUMO interactions).

2.3 Pericyclic reactions in organic synthesis: [1,2] & [2,3] Sigmatropic Rearrangements-Wittig, Mislow-Evans, Stevens and Sommelet-Hauser rearrangements, Sigmatropic rearrangements to cationic centers; Meisen-Heimer Rearrangement.

2.4 [3,3] sigmatropic rearrangements: Cope, Oxy-Cope, aza-Cope, degenerate Cope rearrangements, Carroll rearrangement, Claisen rearrangements.

Suprafacial and antarafacial shifts: [1,3], [1,5], and [1,7] sigmatropic rearrangements, biosynthetic conversion of lumisterol to vitamin D_2, Walk rearrangements, Molecules with "fluxional" structures (bullvalene, homotropilidene etc.).

2.5 FMO analysis of Chelotropic addition, introductory dipolar cycloaddition, Electrocyclic reactions in biological systems: electrocyclizations in the biosynthesis of vitamin D_3.

Textbooks

1. Jagdamba Singh, Jaya Singh, Photochemistry and Pericyclic Reactions, New Age Science Ltd, 3rdEdn., 2009
2. P. S. Kalsi, R. S. Oza, Organic Reactions Stereochemistry and Mechanism - Through Solved Problems, New Age International (P) Ltd., 2018
3. D. Nasipuri, Stereochemistry of Organic Compounds: Principles and Applications, 4th Edn., New Academic Science Ltd., 2012

Reference

1. M. B. Smith, March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure, 7th Edn., Wiley, 2015
2. J. Clayden, N. Greeves, S. Warren, Organic Chemistry, 2nd Edn. Oxford University Press, 2012
3. R. B. Woodward, R. Hoffmann, The Conversation of Orbital Symmetry, 1stEdn., 1971

Module 3: Reactive Intermediates - I (18 hours)

3.1 Carbocations - generation, stability and relative stability(aliphatic and aromatic) and structure- classical and non-classical carbocations- reactions involving carbocation rearrangements like Wagner- Meerwein, Pinacol-pinacolone, Tiffeneau-Demjanov, Dienone phenol, Fries rearrangements.

3.2 Carbanions- generation, stability and relative stability (aliphatic and aromatic) and structure. Reactions of stabilised carbanions like alkynyl anion.

3.3 Structure generation and stability of enolates. Kinetic and thermodynamic enolates- stability and regiochemistry, Enolates from compounds other than carbonyls.

3.4 Knoevenagel and Doebner condensation. Claisen condensation, Dieckmann and Stobbe condensation, Acyloin condensation, Perkin reaction, Darzen reaction, Thorpe reaction. Aldol reaction - inter and intra-molecular aldol condensation, crossed aldol reactions and mixed aldol reaction (stereochemistry not expected). Mukiayama reaction, Imine aldol reaction, Claisen- Schmidt, Condensation reactions of enols and enamines- Mannich reaction- amino methylation, Michael addition-acid and base catalysed and intra molecular, Robinson’s annulations.

Module 4: Reactive Intermediates - II (18 hours)

4.1 Carbenes: Singlet and triplet species- their characteristics, generation, and distinguish between singlet and triplet carbenes - Skell Hypothesis, reactions involving cycloadditions,

C-H insertion, nucleophilic reactions, formation of cyclopropanes, Wolf rearrangement, Diazoketone reactions including Arndt-Eistert reaction, carbenoids.

4.2 Nitrenes: types, generation, structure and reactions like aziridine formation, C-H insertion, Hoffman, Lossen, Curtius and Schmidt rearrangements.

4.3 Free radicals- generation, structure and stability- TEMPO, DPPH radicals, Birch reaction, allylic bromination- NBS and its applications, autoxidation reactions, McMurry coupling. Hofmann-Loffler-Freytag reaction.

4.4 Ylides: chemistry of phosphorous and sulphur ylides – Wittig, Wittig- Hormer, Schlosser modification, Wadsworth- Emmons and related reactions, Arbuzov reaction.

Textbooks (Modules 3 and 4)

1. J. M. Coxon, R. O. C. Norman, Principles of Organic Synthesis, 2nd Edn., Springer, 2012
2. J. Clayden, N. Greeves, S. Warren, Organic Chemistry, 2nd Edn. Oxford University Press, 2012
3. M. B. Smith, J. March, March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure, 6th Edn., Wiley, 2006
4. M. B. Smith, March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure, 7th Edn., Wiley, 2015

Reference (Modules 3 and 4)

1. S. Delvin, Organic Reagents and Name Reactions, Sarup and Sons, 2011
2. Jie Jack Li, Name Reactions, Springer India, New Delhi, 4th Ed. (2011)
3. J. J. Li, Name Reactions: A Collection of Detailed Mechanisms and Synthetic Applications, 5th Edn., Springer Science & Business Media, 2014
4. Penny Chaloner, Organic Chemistry: A Mechanistic Approach, CRC Press, 2014
5. L. Kuerti, B. Czako, Strategic Applications of Named Reactions in Organic Synthesis, Elsevier Academic Press, 2005.
6. M. B. Smith, Organic Synthesis, 3rd Edn., Wavefunctions Inc, 2011.
7. F. A. Carey, R. J. Sundberg, Advanced Organic Chemistry, Part A and B, 5th Edn., Springer, 2007
8. George S Zweifel, Michael H Nantz, Modern Organic Synthesis: An Introduction, 2nd Edn., John Wiley & Sons, 2017
9. Paul Wyatt, Stuart Warren, Organic Synthesis Strategy and Control, John Wiley & Sons, 2013

SEMESTERS I AND II

PRACTICAL

BMCP2P01: INORGANIC CHEMISTRY PRACTICAL - I

Credit: 3 **Total 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 five mixtures containing five different less common ions shall be analysed by a student.

PART II

Colorimetric estimation of Fe, Cu, Ni, Mn, Cr, NH_4^+, nitrate and phosphate ions.

PART III

Preparation and characterization complexes using IR, NMR and electronic spectra.

i. Tris(thiourea)copper(I) complex
ii. Potassium tris(oxalato) aluminate (III)
iii. Hexammine cobalt (III) chloride
iv. Tetrammine copper (II) sulphate
v. Potassium tris(oxalato) chromate (III)
vi. Potassium tris(oxalato) ferrate (III)

PART IV

Mini project

Reference

1. G. Svehla, Vogel's Qualitative Inorganic Analysis, 7th Edn.,Pearson Education India, 2008
2. A.I. Vogel, A Text Book of Quantitative Inorganic Analysis, Longman, 1966
3. I.M. Koltoff, E.B. Sandell, Text Book of Quantitative Inorganic analysis, 3rd Edn., McMillian, 1968
4. V.V. Ramanujam, Inorganic Semimicro Qualitative Analysis, 3rd Edn., The National Publishing Company, 1995

BMCP2P02: ORGANIC CHEMISTRY PRACTICAL-I

Credit: 3 **Total Hours: 54+54=108**

1. Separation of binary and ternary mixtures using chemical and physical methods: Ether, bicarbonate, NaOH, HCl and bisulphite separation.
2. One stage and two stage synthesis
    a. Synthesis of the following (single stage) (some examples)
        i. Methyl orange from sulphanilic acid
        ii. Azobenzene from beta naphthol
        iii. Benzyl alcohol and benzoic acid by Cannizaro's reaction
        iv. Ethyl acetoacetate by Claisen condensation
        v. 1-chloro 2,4-dinitro benzene from chlorobenzene
        vi. 3,5-dinitrobenzoic acid from benzoic acid
        vii. Cinnamic acid by Perkins reaction
    b. Two stage synthesis (some examples)
        i. Aniline-diazoaminobenzene-p-aminoazo benzene
        ii. Benzophenone-oxime-benzanilide (Beckman rearrangement)
        iii. Phthalic anhydride-phthalimide-anthranilic acid (Hofmann rearrangement)
        iv. Acetanilide-parabromoacetanilide-para bromo aniline
        v. Acetanilide-paranitroacetanilide-para nitro aniline
        vi. Chlorobenzene-1-chloro 2,4-dinitrobenzene-2,4-dinitrophenylhydrazine
        vii. Phthalic anhydride-fluorescein-eosin
3. Recording IR and UV spectra of synthesized compounds in sections 1 and 2
4. Chemical Structure drawing using software: Use of structure drawing software to draw the reaction scheme including mechanisms of reactions.
5. Mini project

Reference

1. A.I. Vogel, A Textbook of Practical Organic Chemistry, Longman, 1974
2. A.I. Vogel, Elementary Practical Organic Chemistry, Longman, 1958
3. F.G. Mann, B.C. Saunders, Practical Organic Chemistry, 4thEdn., Pearson Education India, 2009
4. R. Adams, J.R. Johnson, J.F. Wilcox, Laboratory Experiments in Organic Chemistry, Macmillan, 1979

5. N. K. Vishnoi, Advanced Practical Organic Chemistry, 3rd Edn., Vikas Publications, 2013

BMCP2P03: PHYSICAL CHEMISTRY PRACTICAL - I

Credit: 3 **Total Hours: 72+72=144**

I. Adsorption

1. Verification of Freundlich and Langmuir adsorption isotherm: 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.
2. Construction of phase diagram of compounds with congruent melting point: diphenyl amine-benzophenone system.
3. Effect of (KCl/succinic acid) on miscibility temperature.
4. 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 $KI + I_2 \leftrightarrow KI_3$

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.
3. Determination of the composition of binary liquid mixtures (alcohol-water, benzene-nitrobenzene).

VI. Mini project

(Graphs may be drawn manually or using spreadsheets)

Reference

1. J. B. Yadav, Advanced Practical Physical Chemistry, Goel Publishing House, 2001
2. G. W. Garland, J. W. Nibler, D.P. Shoemaker, Experiments in Physical Chemistry, 8th Edn., McGraw Hill, 2009
3. J. H. Jensen, Molecular Modeling Basics, CRC Press, 2010
4. GAMESS documentation available from: http://www.msg.ameslab.gov/gamess/documentation.html

SEMESTER III

BMCP309: MATERIALS CHEMISTRY

Credit: 4 **Total Hours: 72**

Objectives

- To study in detail the essence of solid state chemistry
- To understand the chemistry behind electrical, magnetic and optical properties shown by solids
- To study the methods of preparation and applications of inorganic chains, rings, cages and clusters
- To learn the chemistry of materials such as glass and ceramics

Outcome

At the successful completion of the topics from this course, the student is supposed to get hold of thorough knowledge on:

- various features of structure of solids, solid-state reactions and phase transitions
- prominent theories of solids such as Kronig-Penney model, Free electron theory, Zone theory and MO theory in detail
- the chemistry of superconductivity and its applications
- mode of homogeneous and heterogeneous organometallic catalysis
- applications of various inorganic materials such as inorganic chains, rings, cages, glass, ceramics and clusters

Module 1: Inorganic Photochemistry (9 hours)

1.1 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.

1.2 Metal complex sensitizers-electron relay, semiconductor supported metal oxide systems, water photolysis, nitrogen fixation and CO_2 reduction.

Textbooks

1. V. Balzani, V. Carassiti, Photochemistry of Coordination Compounds, Academic Press, 1970

Reference

1. D.M. Roundhill, Photochemistry and Photophysics of Metal Complexes, Plenum Press, 1994
2. A.W. Adamson, P.D. Fleischauer, Concepts of Inorganic Photochemistry, Wiley, 1975

Module 2: Inorganic Cages and Metal Clusters (9 hours)

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

2.2 Metal clusters: dinuclear compounds of Re, Cu and Cr, metal-metal multiple bonding in $(Re_2X_8)^{2-}$, trinuclear clusters, tetranuclear clusters, hexanuclear clusters. Polyatomic zintl anion and cations. Infinite metal chains.

Textbooks

1. J. E. Huheey, E. A. Keiter, R. L. Keiter, O. K. Medhi, Inorganic Chemistry: Principles of Structure and Reactivity, 4th Edn., Pearson Education, 2006
2. P. Atkins, T. Overton, J. Rourke, M. Weller, F. Armstrong, Inorganic Chemistry, 5th Edn., Oxford University Press, 2010

Reference

1. F. A. Cotton, G. Wilkinson, C. A. Murillo, M. Bochmann, Advanced Inorganic Chemistry, 6th Edn., John Wiley & Sons Inc., 1999
2. K. F. Purcell, J. C. Kotz, Inorganic Chemistry, Holt-Saunders, 1977
3. B. E. Douglas, D. H. McDaniel, J. J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Edn., Wiley-India, 2007
4. R.W. Hay, Bio Inorganic Chemistry, Ellis Horwood, 1984
5. J. D. Lee, Concise Inorganic Chemistry, 5th Edn., Wiley India (P) Ltd., 2010

Module 3: Electrical, Magnetic and Optical Properties (18 hours)

3.1 Kronig-Penney model, Free electron theory, Zone theory and MO theory of solids. Energy bands-conductors and non-conductors, intrinsic and extrinsic semiconductors. Electrons and holes. Mobility of charge carriers. Hall Effect. Pyroelectricity, piezo electricity and ferro electricity. Conductivity of pure metals.

3.2 Magnetic properties of transition metal oxides, garnets, spinels, ilmenites and perovskites, magnetoplumbites.

3.3 Optical properties-photoconductivity, photovoltaic effects, luminescence. Applications of optical properties

3.4 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).Super conducting cuprates - YBaCu oxide system, Meisner effect, conventional superconductors, organic superconductors, fullerenes, carbon nanotubes, high temperature superconductors.

Textbooks

1. L.V. Azaroff, Introduction to Solids, McGraw Hill, 1984
2. A.R. West, Solid State Chemistry and its Applications, Wiley-India, 2007
3. D. K. Chakrabarty, Solid State Chemistry, New Academic Science, 2010

Reference

1. D. M. Adams, Inorganic Solids: An Introduction to Concepts in Solid-State Structural Chemistry, Wiley, 1974
2. C.N.R. Rao, K.J. Rao, Phase Transitions in Solids, McGraw Hill, 2010
3. B. E. Douglas, D. H. McDaniel, J. J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Edn., Wiley-India, 2007
4. A. Earnshaw, Introduction to Magnetochemistry, Academic Press, 1968
5. J. E. Huheey, E. A. Keiter, R. L. Keiter, O. K. Medhi, Inorganic Chemistry: Principles of Structure and Reactivity, 4th Edn., Pearson Education, 2006

Module 4: Applications of Group Theory (27hours)

4.1 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.

4.2 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.

Textbooks

1. K. Veera Reddy, Symmetry and Spectroscopy of molecules, New Age International Publications, 2010

2. F. A. Cotton, Chemical Applications of Group Theory, 3rd Edn., Wiley Eastern, 2008

Reference

1. A. S. Kunju, G. Krishnan, Group Theory and its Applications in Chemistry, 2nd Edn., PHI Learning, 2010
2. V. Ramakrishnan, M. S. Gopinathan, Group Theory in Chemistry, 2nd Edn., Vishal Publications, 2013

Module 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.

Textbook

1. C.V. Agarwal, Chemistry of Engineering Materials, 9th Edn., B. S. Publications, 2006

Reference

1. P.C. Jain, M. Jain, Engineering Chemistry, 12th Edn., Dhanpat Rai Publications, 2006

BMCP310: CONEPTS OF POLYMER CHEMISTRY

Credit: 4 **Total Hours: 72**

Objectives

Awareness about

- polymer science, different types of polymers
- characterisation, mechanism of polymerisation and polymerisation techniques
- knowledge of polymer solutions and theory of polymer solutions
- theoretical insight into the stereochemistry and conformational analysis of polymers

Outcome

On completion of the course, the student shall

- get thorough knowledge of polymer science and different types of polymers
- get expertise in characterisation and mechanism of polymerisation
- appreciable knowledge about polymer solutions and stereochemistry of polymers

Module 1: Introduction to Polymer Science (9hours)

1.1 Polymer science: concepts and terminology. Classification and nomenclature of polymers (with suitable examples) based on origin, structure, backbone, branching, action of heat, ultimate form and use, crystalline and amorphous behaviour. Ladder, semi- ladder and spiropolymers, inorganic polymers.

1.2 Molecular forces in polymers: dipole forces, induction forces, dispersion forces, H-bond.

1.3 Monomers, structure of common polymers like PE, PP, PVC, PVAc, PVA, PMMA, PEMA, polylactic acid, PET, PBT, PTFE, nylon-6, nylon-6,6, Kevlar, PEEK, PES, PC, ABS, PAN, PPO, PEG, SAN, PCL, PLA, PHB, DGEBA, MF, UF, PF, PU, NR, SBR, NBR, PB, butyl rubber, polychloroprene and thiokol rubber, EPDM, CR and polyurethane elastomers.

Module 2: Molecular Weight of Polymers (9hours)

2.1 Polymer molecular weight: different averages, polydispersity index, molecular weight distribution curve, polymer fractionation. Methods for molecular weight determination: end group analysis, colligative property measurements, membrane osmometry, vapour phase osmometry, light scattering, ultracentrifugation, viscometry and GPC.

Textbooks (Modules 1 and 2)

1. V. R. Gowariker, N. V. Viswanathan, J. Sreedhar, Polymer Science, New Age International (P) Ltd., 2011
2. F. W. Billmeyer Jr., Text Book of Polymer Science, 3rd Edn., John Wiley & Sons, 2008
3. J. E. Mark, H.R. Allcock, R. West, Inorganic polymers, 2nd Edn., Oxford University Press, 2005

Reference (Modules 1 and 2)

1. L. H. Sperling, Introduction to Physical Polymer Science, 4th Edn., John Wiley & Sons, 2015
2. P. Ghosh, Polymer Science and Technology: Plastics, Rubber, Blends and Composites., McGraw Hill Education, 2017
3. J. R. Fried, Polymer Science and Technology, 3rd Edn., Prentice Hall, 2014
4. V. Chandrasekhar, Inorganic and Organometallic Polymers, Springer, 2005

Module 3: Mechanisms of Polymerization (18 hours)

3.1 Free radical addition polymerization - mechanism and kinetics of free radical addition polymerization, Chain transfer, Mayo equation, Inhibition and retardation.

3.2 Step reaction (condensation) polymerization-kinetics and mechanism of step reaction polymerization, Carothers equation, number distribution and weight distribution functions, polyfunctional step reaction polymerization, Gelation and gel point.

3.3 Ionic polymerization: common features of the two types of ionic polymerization-mechanism and kinetics of cationic polymerization, expression for the overall rate of polymerization and the number average degree of polymerization, mechanism and kinetics of anionic polymerization, expression for the overall rate of polymerization and the average degree of polymerization, living polymers.

3.4 Ziegler-Natta polymerization: Ziegler-Natta catalysts, mechanism of coordination polymerization-monometallic and bimetallic mechanisms.

3.5 Copolymerization: types of copolymers, the copolymer composition equation, monomer reactivity ratio and copolymer structure, influence of structural effects of monomers on monomer reactivity ratios, the Q-e scheme, synthesis of alternating, block and graft copolymers.

3.6 Atom Transfer Radical Polymerization (ATRP), Reversible Addition Fragmentation Termination (RAFT)

Module 4: Polymerization Techniques (9 hours)

4.1 Bulk polymerization, solution polymerization, suspension polymerization, emulsion polymerization, interfacial condensation.

Module 5: Polymer Solutions (18 hours)

5.1 Solubility of low molecular weight substances and polymers. Theories of polymer solubility, different stages of polymer solubility, non- solvents, solubility of amorphous and crystalline polymers, solubility parameter concept, Hildebrand approach.

5.2 Thermodynamics view of miscibility, LCST , UCST, Lattice theory - advantages and limitations of lattice theory, Flory-Huggins and Flory-Krigbaum theories - advantages and limitation of Flory-Huggins and Flory- Krigbaum theories, corresponding state theories, Flory temperature, polymer-solvent interaction parameter, the unperturbed polymer chain, expansibility factor, entropy, enthalpy and free energy of mixing of polymer solution, phase separation in polymer systems.

5.3 The models of De Gennes and Edwards tube model (worm model), self-avoiding random walk, scaling concepts in polymer systems.

Textbooks (Module 3, 4 and 5)

1. V. R. Gowariker, N. V. Viswanathan, J. Sreedhar, Polymer Science, New Age International (P) Ltd., 2011
2. F. W. Billmeyer Jr., Text book of Polymer Science, 3rd Edn., John Wiley & Sons, 2008
3. G. Odian, Principles of Polymerization, 4th Edn., John Wiley & Sons, 2004
4. K. Matyjaszewski, T.P. Davis, Handbook of Radical Polymerization, Wiley-Interscience, 2002

Reference (Module 3, 4 and 5)

1. P. Ghosh, Polymer Science and Technology: Plastics, Rubber, Blends and Composites., McGraw Hill Education, 2017
2. H. R. Allcock, F. W. Lampe, Contemporary Polymer Chemistry, Prentice Hall, 1981

Module 6: Stereochemistry and Conformation of Polymers (9 hours)

6.1 Positional isomerism in vinyl polymer chains: head to tail, head to head, tail to tail isomerism. Geometrical isomerism in diene polymer chains.

6.2 Configuration of macromolecules: Vinyl polymers with asymmetric centres in the main chain, tacticity and optical isomerism in vinyl polymers, monotactic and ditactic polymers.

6.3 Conformation of macromolecules: tacticity and conformations. Helical conformations. Conformation of macromolecules in the crystals and amorphous solids. Conformation in solutions and melts.

Textbooks

1. F. A. Bovey, Chain Structure and Conformation of Macromolecules, Academic Press, New York, 1982

Reference

1. P. J. Flory, Principles of Polymer Chemistry, Cornell University Press, New York, 1953
2. I. Teraoka, Polymer Solutions: An Introduction to Physical Properties, Wiley, 2004
3. R. J. Young, P. A. Lovell, Introduction to Polymers. 3rdEdn.. CRC Press, 2011
4. D. W. van Krevelen, K. te Nijenhuis, Properties of Polymers: Their Correlation with Chemical Structure; their Numerical Estimation and Prediction from Additive Group Contributions, 4th Edn., Elsevier, 2009

Reference

1. K.J. Saunders, Organic Polymer Chemistry: An Introduction to the Organic Chemistry of Adhesives, Fibres, Paints, Plastics, and Rubbers, Springer Science & Business Media, 2013
2. D.I. Bower, An introduction to Polymer Physics, Cambridge University Press, 2002
3. M. Chanda, Introduction to Polymer Science and Chemistry, A Problem Solving Approach, CRC Press, 2006
4. Data Book on Plastics, Central Institute of Plastics Engineering and Technology, Madras
5. P.G. de Gennes, Scaling Concepts in Polymer Physics, Cornell University Press, 1979

BMCP311: PHYSICAL CHEMISTRY FOR POLYMER SCIENCE

Credit: 4 **Total Hours: 72**

Objectives

The major objectives are

- to give an insight into the kinetics of reactions
- to understand the theory of photochemical techniques
- to study the surface phenomena and catalysis
- to learn advanced topics in electrochemistry

Outcome

After the completion of the course the student shall know

- the kinetics of chemical reactions
- kinetics of photochemical processes and techniques
- the principle of catalysis and surface phenomena
- the DHO equation and related parameters

Module 1: Chemical Kinetics and Catalysis (18 hours)

1.1 Theories of bimolecular reactions: Collision theory-postulates, steric factor, comparison with Arrhenius equation, Activated complex theory- Thermodynamic formulation (Eyring equation) of activated complex theory, Significance of $\Delta G\neq$, $\Delta H\neq$ and $\Delta S\neq$, volume of activation, Statistical formulation of activated complex theory.

1.2 Theories of unimolecular reactions: Lindeman theory (derivation) – Modification of Lindeman theory -Hinshelwood theory (mechanism and qualitative idea), RRK theory (qualitative idea) and RRKM theory (qualitative idea).

1.3 Chain reactions: Free radical and chain reactions, steady state approximation, Rice-Herzfeld mechanism for the kinetics of H_2-Cl_2 and H_2-Br_2 reactions, Semonov-Hinshelwood mechanism of explosive reactions and branching chains H_2-O_2.

1.4 Kinetics of polymerization: Mechanisms of step growth, ionic and addition polymerization, kinetics of anionic and cationic polymerization.

1.5 Fast reactions: Relaxation technique, flow method, shock methods, flash photolysis, NMR technique and ESR methods of studying fast reactions.

1.6 Reactions in solution: Primary kinetic salt effect (Bronsted-Bjerrum theory), secondary kinetic salt effect (qualitative idea), influence of solvent on reaction rates (effect of

dielectric constant, ionic strength and cage effect), primary and secondary kinetic isotope effect, linear free energy relationship (Hammett equation).

1.7 Acid-base catalysis: Specific and general catalysis with examples, Skrabal diagram, Bronsted catalysis law, acidity function.

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

Textbooks

1. K. J. Laidler, Chemical Kinetics, 3rd Edn., Pearson Education India, 2003
2. P. W. Atkins, J.de Paula, Physical Chemistry: Thermodynamics, Structure, and Change, 10th Edn., Oxford University Press, 2014

Reference

1. J.W. Moore, R.G. Pearson, Kinetics and Mechanisms, 3rdEdn., John Wiley & Sons, 1981
2. C. Kalidas, Chemical Kinetic Methods: Principles of Fast Reaction Techniques and Applications, New Age International, 2005
3. J. Rajaram, J.C. Kuriakose, Kinetics and Mechanisms of Chemical Transformations, Macmillan India, 2006

Module 2: Advanced Topics in Computational Chemistry (9 hours)

2.1 Concept of Basis Sets and types; Slater and Gaussian functions; Hartree Fock method, Post Hartree Fock methods (Ab-initio methods), Semi-empirical methods and DFT Methods. (General Introduction only)

2.2 Chemical Computations: Molecular geometry, Cartesian coordinates, internal coordinates, z-matrix, construction of z-matrix with examples. Basic concepts of geometry optimization, single point energy. Koopmans theorem.

2.3 Computational chemistry in chemoinformatics: Fundamental concepts, docking studies. CADD-Computer aided drug designing and its theory- structure activity relationship, Rational drug designing.

Textbooks

1. J. H .Jensen, E. G. Lewars, Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics, 2nd Edn., Springer, 2011
2. F. Jensen, Introduction to Computational Chemistry, 2nd Edn., John Wiley & Sons, 2007

3. A. R. Leach, Molecular Modelling: Principles and Applications, 2nd Edn., Pearson Education Ltd., 2001

Reference

1. J. P. Fackler Jr., L. R. Falvello (Eds.), Techniques in Inorganic Chemistry: Chapter 4, CRC Press, 2011
2. K. I. Ramachandran, G. Deepa, K. Namboori, Computational Chemistry and Molecular Modeling: Principles and Applications, Springer, 2008
3. A. Hinchliffe, Molecular Modelling for Beginners, 2nd Edn., John Wiley & Sons, 2008
4. C.J. Cramer, Essentials of Computational Chemistry: Theories and Models, 2nd Edn., John & Sons, 2004
5. D.C. Young, Computational Chemistry: A Practical Guide for Applying Techniques Real-World Problems, John Wiley & Sons, 2001

Module 3: Electrochemistry and Electromotive Force (27 hours)

3.1 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.

3.2 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.

3.3 Fuel cells, classification based on working temperature, chemistry of fuel cells, H_2-O_2 fuel cells. Lead acid cell and lithium ion cells. Introduction to corrosion and methods of preventing corrosion.

3.4 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.

Textbooks

1. D. R. Crow, Principles and Applications of Electrochemistry, 4th Edn., S. Thornes, 1994
2. B. R. Puri, L. R. Sharma, M. S. Pathania, Principles of Physical Chemistry,47th Edn., Vishal Publishing Co., 2018

Reference

1. S. Glasstone, An Introduction to Electrochemistry, Read Books, 2013

Module 4: Surface Chemistry (9hours)

4.1 Adsorption: Langmuir theory, kinetic derivation, multilayer adsorption-BET theory-derivation, Use of Langmuir and BET isotherms for surface area determination. Application of Langmuir adsorption isotherm in surface catalysed reactions; the Eley-Rideal mechanism and the Langmuir-Hinshelwood mechanism.

4.2 Gibbs adsorption equation (derivation not required), Surface tension, surface films and surface pressure, surfactants and micelles, critical micelle concentration general properties of emulsions.

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

Textbooks

1. A. Goel, Surface Chemistry, Discovery Publishing House, 2006
2. Gurdeep Raj, Surface Chemistry, Goel Publishing House, 2006
3. A. W. Adamson, Physical Chemistry of Surfaces, 6thEdn., John Wiley & Sons Inc., 2000

Reference

1. P. W. Atkins, J.de Paula, Physical Chemistry: Thermodynamics, Structure, and Change, 10th Edn., Oxford University Press, 2014
2. P. W. Atkins, J. de Paula, Physical Chemistry for the Life Sciences, 2ndEdn., Oxford University Press, 2011

Module 5: Photochemistry (9 hours)

5.1 Quantum yield, chemical actinometry, excimers and exciplexes, photosensitization, chemiluminescence, bioluminescence, photo stationary state, dimerization of anthracene (basic idea only), ozone layer in the atmosphere.

5.2 Quenching of fluorescence and its kinetics, Stern-Volmer equation, fluorescence and structure, delayed fluorescence, E-type and P-type.

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

Textbooks

1. N. J. Turro, V. Ramamurthy, J. C. Scaiano, Principles of Molecular Photochemistry: An Introduction, University Science Books, 2009
2. R. J. Silbey, R. A. Alberty, M. G. Bawendi, Physical Chemistry, 4th Edn., John Wiley & Sons, 2005

Reference

1. P. W. Atkins, J.de Paula, Physical Chemistry: Thermodynamics, Structure, and Change, 10th Edn., Oxford University Press, 2014
2. K. K. Rohatgi-Mkukherjee, Fundamentals of Photochemistry, 3rdEdn., New Age International Publishers, 2014
3. C. H. J. Wells, Introduction to Molecular Photochemistry, John Wiley & Sons, 1972
4. Richard P. Wayne, Principles and Applications of Photochemistry, Oxford University Press, 1988

BMCP312: SPECTROSCOPIC METHODS IN ORGANIC CHEMISTRY

Credit: 3 **Total Hours: 54**

Objectives

The objective of this course is to make the student aware of /enable to

- Predict the structure of materials from the spectroscopic data
- Learn the novel techniques used for spectroscopic identification

Outcome

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

- Learn the spectroscopic data of UV/vis, IR, NMR and mass spectral methods
- To elucidate the structure from the spectroscopic data

Module 1: Ultraviolet, Visible and Chiro-optical Spectroscopy (9 hours)

1.1 Energy levels and selection rules, Woodward-Fieser and Fieser-Kuhn rules, Scott's Rule.

1.2 Influence of substituent, ring size and strain on spectral characteristics. Behaviour of benzene and its derivatives, Solvent effect, Stereochemical effect, non-conjugated interactions. Nature of compound from model compounds.

1.3 Chiro-optical properties-ORD, CD, VCD, Cotton effect, octant rule, axial haloketone rule.

1.4 Problems based on the above topics.

Module 2: Infrared Spectroscopy for characterization (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, overtones, Fermi resonance and field effect on frequency, determination of stereochemistry by IR technique.

2.2 IR spectra of organic compounds with common functional groups

2.3 Problems on spectral interpretation with examples.

Module 3: NMR for Materials Chemistry (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, AX_2, AX_3, A_2X_3, AB, ABC, AMX type coupling, first order and non-first order spectra, coupling constant, mechanism of coupling, Karplus curve, 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: basic theory, pulse sequence, COSY, HOMOCOSY, HETEROCOSY basics of HMBC, HSQC, HMQC, 2D-INADEQUATE, J - resolved spectroscopy, NOESY

3.5 Polarization transfer: SPT, SPI, application of DEPT and INEPT, MRI.

3.6 Problems on spectral interpretation with examples.

Module 4: Mass Spectrometry for the Study of Macromolecules (9 hours)

4.1 Molecular ion, base peak, ion production methods (EI). Soft ionization methods: SIMS, FAB, MALDI, TOF, Cyclotron, Field Desorption, Electrospray Ionization. Fragmentation patterns, nitrogen rule, metastable peaks, Mass Analysers: quadrupole, TOF, FTMS, Tandem Techniques, Resolution.

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

4.3 Problems on spectral interpretation with examples.

Module 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).

Textbooks (All modules)

1. D.L. Pavia, G.M. Lampman, G.S. Kriz, Introduction to Spectroscopy, 3rd Edn.,Brooks Cole, 2010
2. Jag Mohan, Organic Spectroscopy: Principles and Applications, 2ndEdn., Narosa, 2010

Reference (All modules)

1. R.M. Silverstein, G.C. Bassler, T.C. Morril, Spectroscopic Identification of Organic Compounds, 7th Edn., Wiley, 2005

2. D. H. Williams, I. Fleming, Spectroscopic Methods in Organic Chemistry, 6th Edn., McGraw-Hill, 2008
3. W. Kemp, Organic Spectroscopy, 3rd Edn., Macmillan, 2008
4. H. Gunther, NMR Spectroscopy, 3rd Edn., Wiley, 2013
5. D. H. Williams, I. Fleming, Spectroscopic Methods in Organic Chemistry, 6thEdn., McGraw-Hill, 2008
6. C. N. Banwell, E.M. McCash, Fundamentals of Molecular Spectroscopy,5th Edn., Tata McGraw Hill, 2017

SEMESTER IV

BMCP413: APPLIED POLYMER SCIENCE

Credit: 3 **Total Hours: 54**

Objectives

The major objectives are to

- provide a background on engineering and speciality polymers
- study the chemistry of adhesives
- provide an awareness on polymer nanocomposites and their applications
- introduce methodologies related to polymer recycling
- introduce various scientific research methods

Outcome

At the end of the course, the students shall

- get thorough knowledge of speciality polymers
- gain expertise in adhesive technology
- get idea about recycling of polymers
- gain the importance of nanotechnology
- get good knowledge for starting a research work

Module 1: Engineering and Speciality Polymers (18 hours)

1.1 Heat resistant and fire resistant polymers: need for heat resistant polymers, improving polymers for high temperature use, need for fire resistant polymers, polymer for low fire hazards, polymers for high temperature resistance, fluoro polymers, aromatic polymers, polyether, polysulphones, polyamides, polyketones.

1.2 Polymers with electrical and electronic properties, conducting polymers- conduction mechanism, applications of conducting polymers, polyacetylene, PPP, polypyrroles and organometallic polymers, photo conducting polymers, polymers in non-linear optics, polymers with piezo, pyro, ferro electric characters, PVDF, trifluroethylene copolymers. Ionic Polymers: classification, types of counter ion and backbone, synthesis, properties and applications. Ionic crosslinking, monomers based on PE, PS, PTFE, polyelectrolytes, ionones.

1.3 Liquid crystalline polymers: definition and synthesis, main chain liquid crystalline polymers, side chain liquid crystalline polymers, combined side chain- main chain liquid crystalline polymers, liquid crystalline polymer networks, liquid crystalline elastomers, biphasic behaviour, structure modification with liquid crystalline polymers, application of liquid crystalline polymers.

Textbooks

1. R.W. Dyson, Specialty Polymers, Chapman and Hall, 2nd Edn., 1998
2. J. M. G. Cowie, Polymers: Chemistry and Physics of Modern Materials, Blackie, London, 1991

Reference

1. H. F. Mark, (Ed), Encyclopedia of Polymer Science and Engineering, John Wiley and Sons, New York, 1989

Module 2: Adhesives (18 hours)

2.1 Adhesives - Concepts and terminology, functions of adhesives, advantages and disadvantages of adhesive bonding, Mechanism of adhesion-mechanical interlocking, inter-diffusion, adsorption and surface reaction, electrostatic attraction.

Wetting and setting,

2.2 Surface treatment, CASING (crosslinking by activated species of inert gas) or plasma treatment, corona discharge, acid etching, transcrystallisation growth, surface grafting, treatment for fluorocarbon polymers and metals.

2.3 Tack and auto adhesion, pressure sensitive adhesion, tackifiers, effects in pressure sensitive adhesion, auto adhesion of elastomers, effect of molecular weight on tack and green strength of NR, effect of contact time and pressure on the tack of elastomers.

2.4 Physical nature of adhesives, hot melt, solutions, aqueous dispersion, activated adhesives, film adhesive, pressure sensitive adhesives, polymerising types, radiation curable.

2.5 Specialty adhesives, adhesives in aerospace, adhesive in automobile industry, adhesives in building construction, adhesive in electrical industry.

Textbooks

1. G. Gierenz, W. Karmann (Editors), Adhesives and Adhesive Tapes, Wiley-VCH, 2001
2. H. R. Allcock, F. W. Lampe, Contemporary Polymer Chemistry, Prentice Hall 1981

Reference

1. J. Shields, Adhesives Handbook, Butterworth-Heinemann, 1985

2. I. Skeist, Handbook of Adhesives, 3rd Edn., Springer-Verlag, 1990
3. E.M. Petrie, Handbook of Adhesives and Sealants, 2nd Edn.,McGraw-Hill Education, 2007
4. A. Pizzi, Wood Adhesives: Chemistry and Technology, Marcel Dekker, 1989

Module 3: Polymers Nanocomposites (6 hours)

Definition of nanocomposites, types of polymer nanocomposites, Synthesis of nanocomposites: Direct mixing, solution mixing, In-situ polymerization

Polymer/Metal oxide nanocomposites, diblock copolymer based nanocomposites, Polymer/CNTs and Polymer/Nanoclay based composites and their properties and functional application.

Textbooks

1. P. M. Ajayan, L.S. Schadler, P. V. Braun, Nanocomposites - Science and Technology, Wiley-VCH, 2004
2. T. J. Pinnavaia, G.W.Beall, Polymer-Clay Nanocomposites, Wiley, 2001

Reference

1. D. L. Chung, Composite Materials, Springer, 2002

Module 4: Polymer Recycling (6 hours)

4.1 Environmental pollution, non-biodegradability of polymers

4.2 SPI coding, Reprocessing of thermoplastic recyclates, contaminants.

4.3 Recycling techniques, size reduction, washing, identification and sorting of plastics, agglomeration, other methods of recycling and waste disposal options, chemical recycling, thermal conversion technologies.

Textbook

1. Introduction to Plastics Recycling, 2nd Edn., Smithers Rapra Technology Ltd., 2007, Vannessa Goodship

Reference

1. Recycling of plastic materials (Ed) Francesco Paolo La Mantia, Chem Tee Publishing.
2. Degradable Polymers, Recycling and Plastics Waste Management, (Eds) Ann Christine Albertsson and Samuel J. Huang, Marcel Dekker, New York.
3. Plastics Waste Management (Ed.) Nabil Mustafa, Marcel Dekkar, New York.

Module 5: Scientific Research Methods (6 hours)

5.1 Meaning of research, types of research, Ethics in research. Source of scientific literature- primary, secondary and tertiary sources, Citation Index, Impact factor, H index, Chemical Abstracts.

5.2 Scientific Writing: Structure of Research paper, thesis and books. Journal articles, communications, reviews etc. Referencing styles. Plagiarism. Peer review process.

Each student is expected to write a short report on any original research paper of their choice and submit during the time of theory viva-voce examination (self work).

Textbooks

1. R. L. Dominoswki, Research Methods, Prentice Hall, 1981
2. J. W. Best, Research in Education, 4th Edn., Prentice Hall of India, 1981
3. H. F. Ebel, C. Bliefert, W. E. Russey, The Art of Scientific Writing, VCH, Weinheim, 1988
4. Joseph, A. Antony, Methodology for Research. Guide for Writing Dissertations, Theses and Scientific Papers, Bangalore: Theological Publications of India, 1986

Reference

1. B. E. Cain, The Basis of Technical Communicating, ACS, 1988
2. H. M. Kanare, Writing the Laboratory Notebook, American Chemical Society, 1985
3. J. S. Dodd, Ed., The ACS Style Guide: A Manual for Authors and Editors; American Chemical Society, 1985
4. J. Gibaldi W. S. Achtert, Handbook for writers of Research Papers; 2nd Edn.; Wiley Eastern, 1987

ELECTIVE COURSES

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

BMCP4E01: PROPERTIES AND CHARACTERIZATION OF POLYMERS

Credit: 3 **Total Hours: 72**

Objectives

The objective of this course is to

- Understand the morphology and theories of crystalline polymers
- study the flow properties of polymeric materials
- acquaint with chemical reactions, degradation mechanisms, and polymers in peptide synthesis
- familiarise with the structural testing and characterisation of polymers

Outcome

At the end of the course, the student shall

- Learn the morphology and crystallinity of polymers
- understand the viscoelastic properties of polymeric materials
- understand the degradation mechanisms of polymers
- interpret the results of physical property characterisation techniques

Module 1: Polymer Morphology (18 hours)

1.1 Amorphous state, First order and second order transitions, T_g, T_m, factors affecting T_g, free volume, kinetic and thermodynamic views of glass transition, internal and external plasticisation, determination of T_g.

1.2 Polymer morphology: common polymer morphologies, structural requirements for crystallinity, degree of crystallinity, crystallisability - mechanism of crystallization.

1.3 Polymer single crystals: lamellar structure of polymers - fringed micelle concept, folded chain model, adjacent re-entry model, switchboard model. Structure of polymers crystallized from melt - super crystalline structures, spherulites.

1.4 Theories of crystallization - Avrami equation, Hoffman's nucleation theory, the entropic barrier theory. Strain induced morphology, cold drawing, morphology changes

during orientation. Theory and application of XRD, SEM and DSC in determining the crystallinity of polymers.

Textbooks

1. F. W. Billmeyer Jr., Text book of Polymer Science, 3rd Edn., John Wiley & Sons, 2008
2. V. R. Gowariker, N. V. Viswanathan, J. Sreedhar, Polymer Science, New Age International (P) Ltd., 2011

Reference

1. L. H. Sperling, Introduction to Physical Polymer Science, 4th Edn., John Wiley & Sons, 2015
2. M. Chanda, Introduction to Polymer Science and Chemistry: A Problem Solving Approach, 2ndEdn., CRC Press, 2006
3. J.M.G. Cowie, V. Arrighi, Polymers: Chemistry and Physics of Modern Materials, 3rd Edn., CRC Press, 2007

Module 2: Polymer Viscoelasticity and Rheology (18 hours)

2.1 Polymer viscoelasticity, introduction to the viscoelastic properties of polymers, some simple linear viscoelastic models - Maxwell model, Voigt model, generalized linear viscoelasticity, Boltzmann principle, linear viscoelastic behaviour of polymer solids, creep experiments, stress relaxation experiments, stress-strain experiments, oscillatory experiments, dynamic mechanical analysis, elastic modulus, time temperature equivalence, time-temperature superposition principle, WLF equation, Introduction to rubber elasticity, molecular requirements of rubber like elasticity, thermodynamics of rubber elasticity.

2.2 Rheological properties of polymers - introduction to polymer melt rheology, Newtonian fluids, non-Newtonian fluids, pseudoplastic, dilatant, complex rheological fluids, thixotropic and rheopectic fluids, time dependent fluids, time independent fluids, power law, Weissenberg effect, laminar flow, turbulent flow, die swell, shark skin, viscous flow, melt flow index, Cone-and-Plate Rheometer, Capillary Rheometer

Textbooks

1. F. W. Billmeyer Jr., Text book of Polymer Science, 3rd Edn., John Wiley & Sons, 2008
2. V. R. Gowariker, N. V. Viswanathan, J. Sreedhar, Polymer Science, New Age International (P) Ltd., 2011
3. H. R. Allcock, F. W. Lampe, Contemporary Polymer Chemistry, Prentice Hall, 1981

4. J. A. Brydson, Flow Properties of Polymer Melts, Godwin in Association with the Plastics and Rubber Institute, 1981

Reference

1. David J. Williams, Polymer Science and Engineering, Maclaren and Sons, New York, 1978
2. H. F. Haufman, J. J. Falcetta, Introduction to Polymer science and Technology, S P E Text Book, John Wiley & Sons New York 1997
3. A. V. Tobolsky, Properties & structure of polymers, John Wiley & Sons New York 1960
4. R. J. Samuels, Structured Polymer Properties, John Wiley & Sons, New York, 1974
5. J. D. Ferry, Viscoelastic Properties of Polymers, John Wiley & Sons New York 1971

Module 3: Polymer Reactions and Degradation (9 hours)

3.1 Polymer Reactions: hydrolysis, acidolysis, aminolysis, crosslinking, addition and substitution reactions, cyclisation reactions.

3.2 Chain end and random degradation, degradation by oxygen, ozone, heat, UV light, microorganisms. Crazing, weathering, stabilization to prevent degradation.

3.4 Polymeric reagents - Polymers as supports in solid phase peptide synthesis: a detailed survey of the various polymeric supports, their merits and limitations in the solid phase synthesis strategy.

Textbook

1. V. R. Gowariker, N. V. Viswanathan, J. Sreedhar, Polymer Science, New Age International (P) Ltd., 2011

Reference

1. Paul C. Painter and Michael M. Coleman, Fundamentals of Polymer Science, Technomic Publishing Co. Inc., Lancaster, USA, 1994
2. Ulf W Gedde, Polymer Physics, Chapman & Hall, 1995
3. D. W. Van Krevelen, P. J. Hoftyzen, Properties of Polymer, 3rd Edition Elsevier Scientific Publishing Company, New York. 1990
4. J. E. Mark (Ed.) AIP, Physical Properties of Polymers Hand Book, Williston, Vt, 1996.
5. Jozef Bicerano, Prediction of Polymer Properties, 2nd Edn, Marcel Dekker, New York, 1995.

Module 4: Polymer Testing and Characterization (27 hours)

4.1 Thermal analysis such as dilatometry, TMA, DSC, DTA, TGA and DTG. Spectroscopic techniques such as FTIR, NMR, EPR, Raman, UV-visible, Fluorescence and X-ray diffraction.

4.2 Mechanical properties-stress, strain, elongation, yield point, yield strength, proportional limit, modulus of elasticity, ultimate strength, secant modulus, stress- strain behaviour of different types of polymers, tensile strength, tension compression, flexure, elongation at break, modulus, tear strength, hardness, impact properties, creep, stress-relaxation, abrasion, fatigue resistance.

4.3 Thermal properties-specific heat, heat deflection temperature, thermal conductivity, thermal expansion, brittleness temperature.

4.4 Electrical Properties: dielectric strength, dielectric constant, dissipation factor, electrical resistance, volume resistivity and surface resistivity, arc resistance.

4.5 Optical Properties: optical clarity, colour assessment, refractive index, luminous transmittance, haze and gloss, total internal reflection, birefringence.

Textbooks

1. Vishu Shah, Handbook of Plastics Testing and Failure Analysis, 3rdEdn., Wiley-Interscience, 2007.

Reference

1. R. P. Brown, Physical testing of Rubber, Academic Press, New York 1984

BMCP4E02: POLYMER SCIENCE AND TECHNOLOGY

Credit: 3 **Total Hours: 72**

Objectives

The objectives of this course are to make the student aware of

- Polymer blends and composites
- fibre science
- latex technology
- various polymer processing techniques

Outcome

At the end of the course, the student shall

Describe and distinguish between polymer blends and composites

- Understand blend and composite technology
- Learn the nomenclature, classification, composition, production and applications of various natural and man-made fibres.
- Learn latex technology and applications
- learn various polymer processing techniques

Module 1: Polymer Compounding (18 hours)

1.1 Additives for compounding plastics, fillers, plasticizers and softeners, lubricants and flow promoters, antiaging additives, flame retarders, colorants, blowing agents, UV stabilizers, requirement and functions of ingredient.

1.2 Compounding ingredients for rubber: Fillers-reinforcing, semi- reinforcing and non-reinforcing, peptizers, vulcanizing agents, activators, accelerators, anti-oxidants, antiozonants, pigments, tackifiers, blowing agents, bonding agents and processing aids. Vulcanization of rubber, types of vulcanisation, rheograph, cure time, scorch time.

1.3 Compound development-formulation of mixes, basic recipe, typical formulations, Tire Carcass compound-Tire tread- Automobile bushes-Bridge bearing pads- Rubber band-Footwear soles-Floor tiles- Wiper blade- Washing machine gasket- Pressure cooker gasket-O-rings.

Textbooks

1. Claude M. Blow, Claude Hepburn, Rubber Technology and Manufacture, Elsevier Science & Technology Books, 1982.

2. Howard L. Stephens, Krishna C. Baranwal, Basic Elastomer Technology, Rubber Division, American Chemical Society, 2001.
3. C.W. Evans, Practical Rubber Compounding and Processing, Elsevier, 1981

Reference

1. Anil K. Bhowmick, Malcom M Hall, Henry A Benarey, Eds., Rubber Products Manufacturing Technology, Marcel Dekker, 1994.

Module 2: Latex Technology (9 hours)

2.1 Introduction to latices, classification of latices, comparisons and contrasts between polymer latices and polymer solutions, investigation of latex properties- TSC, DRC, pH, alkalinity, colloidal stability, KOH number, VFA, surface free energy, density, residues. Preservation and concentration of natural rubber latex, dipping methods, manufacturing of gloves, rubber bands, balloons, latex casting, latex foam, manufacturing of latex thread.

Textbooks

1 R. Joseph, Practical Guide to Latex Technology, Smithers Rapra Technology Ltd, 2013

2 A.K. Bhowmick, M.M Hall, H.A. Benarey, Eds., Rubber Products Manufacturing Technology, Marcel Dekker, 1994

Reference

1 D. Hill, Science and Technology of Latex Dipping, Smithers Rapra Technology, United Kingdom, 2018

Module 3: Polymer Processing (9 hours)

3.1 Processing methods for the manufacture of products with dry rubber-blending and mastication, master batching of polymers, mixing and compounding in mills and internal mixers, calendaring, sheeting, fabric coating, extension, moulding, batch curing, cold curing, continuous vulcanization methods-high pressure steam, hot air tunnel, molten salt bath, fluidized bed, continuous drum care and microwave curing.

3.2 Processing methods of plastics-methods of mixing-injection, reaction injection, compression and transfer moulding, extrusion, calendaring, thermoforming, blow moulding, rotational moulding and slush moulding.

Textbooks

1. G.J. Morton-Jones, Polymer Processing, Springer Netherlands, 1989

2. V. R. Gowariker, N. V. Viswanathan, J. Sreedhar, Polymer Science, New Age International (P) Ltd., 2011

Reference

1. D.V. Rosato Kluwer, Injection moulding handbook. - Academic Publishers Boston 2nd edtion 1995.
2. Richard C. Progelhof James. L. Throne, Polymer Engg. Principles, Hanser Publisher Munich 1993
3. N.P. Charemisinoff & P.N. Chere, Handbook of applied Polymer Processing Tech, Marcel Dekker, inc, NY 1996.
4. Herbert Recs, Understanding of Injection moulding Tech., Hanser Pub., Munich 1994.

Module 4: Manufacturing of Polymers (9 hours)

4.1 Production, properties and applications of LDPE, HDPE, PS, PC, PVC, PMMA, SBR, NBR.

Textbooks

1. J.A. Brydson, Plastic Materials, Butterworths-Hieneman, 1999

Reference

1. K. J. Saunders, Organic Polymer Chemistry, Chapman and Hall, London.1973

Module 5: Polymer Blends and Composites (18 hours)

5.1 Introduction, preparation of polymer blends, Solution mixing, Mechanical mixing, Latex blending, Mechanochemical blending

452 Thermodynamic criteria for polymer miscibility, phase separation, spinodal decomposition, nucleation and growth, phase diagram,

5.3 Methods for determining polymer-polymer miscibility,

454 Compatibilisation-fundamental concepts, general routes to compatibility, types of compatibilisers-addition of graft of block copolymers, insitu formed copolymers, separately added copolymers, reactive compatibilisation by low molecular weight additives,

5.5 Rubber plastic blends, dynamic vulcanization, thermoplastic elastomers, thermoplastic styrene block copolymers, polyester TPEs, thermoplastic PU elastomers.

5.6 Polymer composites: definition and classification, role of fibre and matrix, mechanics of short and long fibre composites, effect of coupling and bonding agents, critical fibre length in short fibre composites, rule of mixtures, polymer concrete

5.7 Introduction to resins (polyester, epoxies, phenolics) and reinforcements (glass, carbon, aramid, polyester, nylon), moulding process – hand layup, spray up, filament winding, vacuum bag moulding, pressure bag moulding, resin transfer moulding, pultrusion.

Textbooks

1. O. Olabisi, L.M. Robeson, M.T. Shaw, Polymer-Polymer Miscibility, Academic Press, 1979
2. D.R. Paul, Polymer Blends, Vol. 1 and Vol. 2, Academic Press, 1978
3. K. K. Chawla, Composite Materials: Science and Engineering, Springer, 1998.

Reference

1. F. R. Jones, Hand Book of Polymer-Fibre Composites, Longman Scientific and Technical, 1994.
2. Brent A Strong, Fundamentals of Composites Manufacturing: Materials, Methods and Applications, Society of Manufacturing Engineers, 1989

Module 6: Fibre Science and Technology (9 hours)

6.1 Definition of fibres, classification and nomenclature of fibres, structural principles of fibre forming polymers.

6.2 Chemical composition, and use of vegetable fibres such as cotton, flax, linen, coir, sisal, animal fibre such as wool and silk, mineral fibre such as asbestos and glass.

6.3 Chemical composition, production and properties of man-made fibres such as viscose, rayon, nylon-6,6, nylon-6, carbon fibre, polyesters, acrylic fibres.

6.4 Fibre spinning methods (melt, wet and dry spinning), after treatments, fibre drawing, heat setting, applications of fibres in rubber and plastic industries.

Textbooks

1 P. Ghosh, Fibre Science and Technology, Tata McGraw-Hill Education, 2004

2 S. P. Mishra, A Text Book of Fibre Science and Technology, New Age International Publishers, 2005

Reference

1 R.W. Moncrieff, Man-made Fibres, Wiley Interscience, 1970

2 F. W. Billmeyer Jr., Text book of Polymer Science, 3rd Edn., John Wiley & Sons, 2008

3 R.M. Kozłowski (Ed.), Handbook of Natural Fibres: Processing and Applications, Woodhead Publishing Limited, 2012

BMCP4E03: SYNTHETIC ORGANIC CHEMISTRY

Credit: 3 **Total Hours: 72**

Objectives

The main objectives of this paper is to

- Study various oxidation and reduction methods
- Know retrosynthetic analysis of organic compounds
- Understand about the use of protecting groups in synthesis
- Analyse various photochemical reactions
- To synthesise various carbocyclic compounds

Outcome

The expected outcome are

- Students will be able to design various synthesis using oxidation and reduction agents, protecting group and retrosynthetic methods
- Can effectively use light for organic reactions
- Can design various reactions for cyclic compounds

Module1: Oxidation and Reduction Methods in Organic Chemistry (18 hours)

1.1 Oxidation: Metal based and non-metal based oxidations of

(a) alcohols to carbonyls using Chromium, DMSO, TEMPO based reagents, Jones, Collins-Ratcliff reagents, PCC, PDC, Swern oxidation, Dess- Martin Periodinane oxidation-DMP, tetrapropylammonium perruthenate-TPAP.

(b) phenols (Fremy's salt, silver carbonate on Celite (Fetizon's reagent))

(c) alkenes to epoxides (peracids based epoxidation – with special reference to peracid reactivity, stereoselectivity and chemoselectivity)

(d) alkenes to diols: Prevost and Woodward hydroxylation

(e) alkenes to carbonyls with bond cleavage: Ozonolysis

(f) alkenes to alcohols/carbonyls without bond cleavage (hydroboration-oxidation, Wacker Oxidation, Selenium based oxidation)

(g) ketones to ester/lactones (Baeyer-Villiger oxidation, Babler oxidation)

1.2 Reduction: Metal based and non-metal based reductions

(a) Catalytic hydrogenation using Palladium based catalysts, Noyori asymmetric hydrogenation

(b) Metal based reductions: Birch reduction, Pinacol formation, McMurray coupling, Acyloin formation, dehalogenation and deoxygenations.

(c) Hydride transfer reagents from Group III and Group IV in reductions.

i. $NaBH_4$, L-selectride, K-selectride, Luche reduction; $LiAlH_4$, DIBAL-H, Trialkylsilanes and Trialkylstannane.

ii. Stereo/enantioselective reductions involving 9-BBN, $(Sia)_2BH$, Corey-Bakshi-Shibata catalyst.

Textbooks

1. F. A. Carey, R. J. Sundberg, Advanced Organic Chemistry, Part A and B, 5th Edn., Springer, 2007
2. M. B. Smith, March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure, 7th Edn., Wiley, 2015

Reference

1. R. E. Gawley, J. Aube, Principles of Asymmetric Synthesis, 2nd Edn., Elsevier Ltd., 2012
2. P. S. Kalsi, Organic Reactions and Their Mechanisms, New Age Science Ltd., 2017
3. W. Carruthers, Modern Methods of Organic Synthesis, 4th Edition, Cambridge University Press, 2015
4. T. Okuyama, H. Maskill, Organic Chemistry: A Mechanistic Approach, Oxford University Press, 2014
5. J. M. Coxon, R. O. C. Norman, Principles of Organic Synthesis, 2nd Edn., Springer, 2012

Module 2: Organic Reagents and Protecting Groups (9 hours)

2.1 Protection and deprotection of amino, carboxylic acid, carbonyl, and hydroxyl groups.

2.2 Reagents- Dicyclohexyl carbodiimide (DDC), 1,3-Dithiane (Umpolung reagent), DDQ, Trimethylsilyl iodide- Petersons reaction, Gilman Reagent, Polymer supported reagents, NBS.

Textbooks

1. Jagdamba Singh, L. D. S. Yadav, Organic Synthesis, Pragati Prakashan, 2014
2. J. M. Coxon, R. O. C. Norman, Principles of Organic Synthesis, 2nd Edn., Springer, 2012

Reference

1. F. A. Carey, R. J. Sundberg, Advanced Organic Chemistry, Part A and B, 5th Edn., Springer, 2007
2. M. B. Smith, Organic Synthesis, 4th Edition, Academic Press, 2016
3. W. Carruthers, Modern Methods of Organic Synthesis, 4th Edition, Cambridge University Press, 2015

Module 3: Disconnection Approach in Organic Synthesis (9 hours)

3.1 Basic principles and terminology of retrosynthesis, important strategies of retrosynthesis. Important functional group interconversions. one group and two group C-X and C-C disconnections, amine and alkene synthesis and aromatic compounds(At least 40 compounds to be worked up followed by forward synthesis).

Textbooks

1. S. Warren, Organic Synthesis, The disconnection Approach, John Wiley & Sons, 2004

Reference

1. Ratan Kumar Kar, Fundamentals of Organic Synthesis: The Retrosynthetic Analysis, NCBA Publishers, 2007
2. J. M. Coxon, R. O. C. Norman, Principles of Organic Synthesis, 2nd Edn., Springer, 2012

Module4: Metal Mediated Reactions in Organic Synthesis (18 hours)

4.1. Use of organolithium agents: Preparation, reactivity, lithium halogen exchange, transmetalation, metalation, chemoselectivity, benzilic and allylic metallation, metalltion of alpha –heteroatom substituted alkenes and 1-alkynes, conjugate addition.

4.2 Organo magnesium reagents: Grignard Reagents- preparation and reactions, Kumada coupling.

4.3 Organotitanium reagents: Tebbe olefination, Zeigler's reagent.

4.4 Organocopper reagents: Preparation and reaction of organic cuprates. Preparations of enones Conjugate addition, Tandem 1,4- addition by enolate trapping, O trapping, C trapping.

4.5 Organo chromium reagents: Nosaki-Hiyama Reaction, Nozaki Takai Hiyama Kishi Coupling.

4.6 Organo zinc reagents: Preparation and reactions- Reactions of functionally substituted RZnI.

4.7 Organo boron reagents: carbonylation, synthesis of ketones and tertiary alcohols, cyanidation, dichloromethyl ether reaction, Matteson's Boronnic Ester homologation, Brown's asymmetric Crotylboration.

4.8 Palladium catalysed coupling reactions: General considerations, Mizoroki-Heck reaction, palladium catalysed cross coupling reactions like - Negishi type reactions of coupling with organo aluminum, organo zinc and organo zirconium compounds, Suzuki-Miyaura coupling, Stille coupling, Buchwald-Hartwig reaction.

4.9 Cross coupling involving sp carbons: Castro- Stephens reaction, preparation of conjugated enediynes, 1,3-diynes, Trost- Tsuji reaction.

Textbooks

1. J. M. Coxon, R. O. C. Norman, Principles of Organic Synthesis, 2nd Edn., Springer, 2012

Reference

1. George S Zweifel, Michael H Nantz, Modern Organic Synthesis: An Introduction, 2nd Edn., John Wiley & Sons, 2017
2. Paul Wyatt, Stuart Warren, Organic Synthesis Strategy and Control, John Wiley & Sons, 2013

Module 5: Photochemical Reactions (9 hours)

5.1 Photochemistry of (π - π^*) transitions: Excited states of alkenes, cis-trans isomerisation, electrocyclisation and sigmatropic rearrangements, di-π methane rearrangement. Photocycloadditions of simple and conjugated olefins.Photochemistry of alkynes.

5.2 Photochemistry of aromatic compounds: Ring isomerization, cycloaddition, nucleophilic substitution and cyclization reactions.

Photochemistry of (n-π^*) transitions: Excited states of carbonyl compounds, homolytic cleavage of α- bond, Norrish type I reactions in acyclic and cyclic ketones. Photo Fries rearrangements. Intermolecular abstraction of hydrogen- photoreduction of ketones, Intramolecular abstraction of hydrogen- Norrish type II reactions in ketones, Paterno-Buchi reaction and Barton reaction.

5.3 Intermolecular abstraction of hydrogen: photoreduction of ketones, Intramolecular abstraction of hydrogen:Norrish type II reactions in ketones and esters, Addition to carbon-carbon multiple bonds, Paterno-Buchi reaction, Photochemistry of nitrites-Barton reaction.

Textbooks

1. J. D. Coyle, Introduction to Organic Photochemistry, John Wiley & Sons Ltd., 1991

2. N. J. Turro, V. Ramamurthy, J. C. Scaiano, Principles of Molecular Photochemistry: An Introduction, University Science Books, 2009

Reference

1. N. J. Turro, V. Ramamurthy J. C. Scaiano, Modern Molecular Photochemistry for Organic Molecules, Viva books, 2017
2. R. Kumar, V. P. Sharma, Pericyclic Reactions and Organic Photochemistry, Reprint, Pragati Prakashan, 2018
3. P. Kl´an, J. Wirz, Photochemistry of Organic Compounds: From Concepts to Practice, 1st Edn., Wiley-Blackwell, 2009

Module 6: Construction of Carbocyclic Rings (9 hours)

6.1 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.

6.2 Inter-conversion of ring systems (contraction and expansion)-Demjenov reaction, Reformatsky reaction. Construction of macrocyclic rings-ring closing metathesis.

6.3 Inter and Intramolecular Paterno-Buchi reaction: synthetic applications - preparation of Azulene. Introduction to metathesis reactions

Textbooks

1. J. M. Coxon, R. O. C. Norman, Principles of Organic Synthesis, 2nd Edn., Springer, 2012
2. Goutam Brahmachari, Organic Name Reactions: Narosa Publishing House, 2007

Reference

1. D. Nasipuri, Stereochemistry of Organic Compounds: Principles and Applications, 4th Edn., New Academic Science Ltd., 2012
2. Robert H. Grubbs, Anna G. Wenzel (Eds.), Handbook of Metathesis: Catalyst Development and Mechanism, 2nd Edition Wiley, 2013
3. Jagdamba Singh, Jaya Singh, Photochemistry and Pericyclic Reactions, New Age Science Ltd, 3rd Edn., 2009
4. R. Kumar, V. P. Sharma, Pericyclic Reactions and Organic Photochemistry, Pragati Prakashan, 2018

BMCP4E04: MODERN ANALYTICAL INSTRUMENTATION

Credit: 3 **Total Hours: 72**

Objectives

The main objectives of this course are

- familiarising important electroanalytical techniques
- to obtain basic knowledge on thermoanalytical methods, chromatography, electrochromatography etc.

Outcome

After the successful completion of the course the student shall knew

- various elelctroanalytical techniques
- the significance of capillary electrophoretic techniques
- the significance and principle of thermal methods of analysis
- expanded bed chromatographic separation and its applications

Module 1: Electro Analytical Methods (27 hours)

1.1 Potentiometry: techniques based on potential measurements, direct potentiometric systems, different types of indicator electrodes, limitations of glass electrode, applications in pH measurements, modern modifications, other types of ion selective electrodes, solid, liquid, gas sensing and specific types of electrodes, biomembrane, biological and biocatalytic electrodes as biosensors, importance of selectivity coefficients. Chemfets-importance of specially designed amplifier systems for ion selective electrode systems.Potentiometric titrations-types and applications.

1.2 Polarography and voltametric techniques: micro electrode and their specialities, potential and current variations at the micro electrode systems, conventional techniques for concentration determination, limitations of detection at lower concentrations, techniques of improving detection limit-rapid scan, ac, pulse, differential pulse square wave polarographic techniques. Applications of polarography.

1.3 Amperometry: biamperometry, amperometric titrations. Coulometry-primary and secondary coulometry, advantages of coulometric titrations, applications. Principle of chronopotentiometry. Anodic stripping voltammetry-different types of electrodes and improvements of lower detection limits. Voltammetric sensors. Organic polarography.

Textbook

1. D. A. Skoog, F. J. Holler and S. R. Crouch, Principles of Instrumental Analysis, 7th Edn., Cengage Learning, 2017

Reference

1. G. D. Christian, J. E. O'Reilly, Instrumental Analysis, Allyn and Bacon, Inc., 1986
2. F. A. Settle, Handbook of Instrumental Techniques for Analytical Chemistry, Prentice Hall, 1997
3. H. H. Willard, L. L. Merritt, J. A. Dean, F. A. Settle, Instrumental Methods of Analysis, 7th Edition, CBS Publishers and Distributors, 2018

Module 2: **Capillary Electrophoresis and Capillary Electro Chromatography (9 hours)**

2.1 Capillary electrophoresis- Theory, electrophoretic mobility, electroosmotic mobility, factors affecting migration of ions, migration time, plate heights, selectivity and resolution. Instrumentation: sample introduction, detection methods and applications. Modes of capillary electrophoresis: Capillary zone electrophoresis (CZE), Capillary isotachophoresis, Isoelectric focusing. Capillary gel electrophoresis.

2.2 Capillary electro chromatography-packed columns, mobile phase, sample injection, detection and applications. Micellar electro kinetic chromatography-theory and applications.

Textbooks

1. F. Rouessac, A. Rouessac, Chemical Analysis: Modern Instrumentation Methods and Techniques, 2ndEdn., John Wiley & Sons, 2007

Reference

1. K. D. Altria, Capillary Electrophoresis Guidebook. Principles, Operation, and Applications, 1stEdn., Humana Press, 1996
2. R. Weinberger, Practical Capillary Electrophoresis 2nd Edn., Academic Press, 2000
3. S. F. Y. Li, Capillary Electrophoresis: Principles, Practice, and Applications, 1st Edn., Elsevier Science, 1992

Module 3: Thermal Methods of Analysis (9 hours)

3.1 Theory, instrumentation and application of (i) Thermogravimetric Analysis (TGA), (ii) Differential Thermal Analysis (DTA), (iii) Differential Scanning Calorimetry (DSC), (iv) Thermomechanical analysis (TMA) and (v) Dynamic mechanical analysis (DMA); - Thermograms of above techniques, information from thermograms, factors affecting

thermograms and applications of thermograms for qualitative/quantitative analysis. Thermometric titrations– theory, applications.

Textbooks

1. M. E. Brown, Introduction to Thermal Analysis: Techniques and Applications, Springer, 2001
2. R. F. Speyer, Thermal Analysis of Materials, CRC Press, 1993

Reference

1. T. Hatakeyama, F.X. Quinn, Thermal Analysis: Fundamentals and Applications to Polymer Science, 2nd Edn., John Wiley & Sons, 1999
2. Principles of Thermal Analysis and Calorimetry, Edited by P. J. Haines, RSC paperbacks, 2002
3. Principles and Applications of Thermal Analysis, Edited by P.Gabbott, Blackwell Publishing, 2008
4. P.J. Haines, Thermal Methods of Analysis: Principles, Applications and Problems, Springer, 1995

Module 4: Chromatography (18 hours)

4.1 Classification of chromatography: Gas chromatography, GSC and GLC Instrumentation, different types of detectors, capillary columns-bonded and crosslinked phases, chiral stationary phases, factors affecting Gas chromatography, selectivity factors, applications.

4.2 Liquid Chromatography: column efficiency, band broadening and the factors affecting it, particle size. HPLC-its instrumentation pumps, sample injection, columns, solvent selection and detectors.

4.3 Ion exchange chromatography-ion exchange equilibria, packings, detectors, applications.

4.4 Size exclusion chromatography - columns and limits of permeation and exclusion, applications.

4.5 Planar Chromatography-methodology, materials for stationary phases, applications. Paper chromatography and TLC

4.6 Supercritical fluid chromatography: properties of supercritical fluids, operating variables in instrumentation, stationary and mobile phases, advantages and applications.

4.7 Expanded bed chromatographic separation: Technique and applications

Textbooks

1. J. G. Dick, Analytical Chemistry, R. E. Krieger Pub., 1978
2. G. D. Christian, J. E. O'Reilly, Instrumental Analysis, Allyn and Bacon, Inc., 1986

Reference

1. J. H. Kennedy, Analytical Chemistry: Principles, Saunders College Pub., 1990
2. C. L. Wilson, D.W. Wilson, Comprehensive Analytical Chemistry, Elsevier, 1982
3. A. I. Vogel, A Textbook of Practical Organic Chemistry, Longman, 1974
4. F. W. Fifield, D. Kealey, Principles and Practice of Analytical Chemistry, Blackwell Science, 2000

Module 5: Surface Study Techniques - Instrumentation and Applications (9 hours)

5.1 Spectroscopic methods: ISS, SIMS, ESCA, AES, AAS.

5.2 Microscopic methods: SEM, STM, AFM, TEM.

Textbooks

2. D. A. Skoog, F. J. Holler and S. R. Crouch, Principles of Instrumental Analysis, 7th Edn., Cengage Learning, 2017

Reference

1. G.D. Christian, J.E. O'Reilly, Instrumental Analysis, Allyn and Bacon, Inc., 1986
2. F.A. Settle, Handbook of Instrumental Techniques for Analytical Chemistry, Prentice Hall, 1997
3. H.H. Willard, L.L. Merritt, J.A. Dean, F.A. Settle, Instrumental Methods of Analysis, 7thEdn., CBS Publishers and Distributors, 2018

SEMESTERS III AND IV

PRACTICAL

BMCP4P04: POLYMER PREPARATIVE PRACTICAL

Credit: 3 **Total Hours: 108**

PART I: Preparation of Polymers

Any six preparation of the following (preparations are only illustrative, same or similar may be carried out)

1. Preparation of glyptal resin
2. Preparation of phenol formaldehyde resin (resoles and novolaks)
3. Preparation of urea formaldehyde resin
4. Preparation of aniline formaldehyde resin
5. Preparation of polyaniline
6. Regeneration of cellulose
7. Preparation of nylon -6,6 (interfacial polycondensation)
8. Preparation of PMMA (free radical bulk polymerisation)
9. Preparation of polyacrylamide (free radical polymerisation)
10. Preparation of polyacrylamide (redox polymerisation)
11. Preparation of linear polystyrene (free radical polymerisation)
12. Preparation of crosslinked polystyrene (suspension polymerisation)

PART II: Latex Analysis

1. Determination of total solid content of latex
2. Determination of alkalinity of latex
3. Determination of dry rubber content of latex
4. Determination of volatile fatty acid number of latex
5. Determination of viscosity of latex
6. Determination of KOH number
7. Determination of coagulum
8. Determination of sludge
9. Determination of mechanical stability time (MST)

10. Determination of specific gravity
11. Magnesium content

Reference

1. E.A. Collins, J. Bares, F.W. Billmeyer, Experiments in Polymer Science, Wiley-Interscience, 1973
2. S.H. Pinner, A Practical Course in Polymer Chemistry, Pergamon, 1961
3. D. Braun, H. Cherdron, W. Kern, Practical Macromolecular Organic Chemistry, 3rdEdn., Harwood Academic Publishers,1984
4. S.R. Sandler, W. Karo, Polymer Synthesis, Vol.1, Academic Press, 1992
5. S.R. Sandler, W. Karo, Polymer Synthesis, Vol.2, Academic Press, 1993
6. S.R. Sandler, W. Karo, Polymer Synthesis, Vol.3, Academic Press, 1998
7. D. C. Blackley, Polymer Latices, Vol.1, 2 & 3, 2nd Edn., Springer, 1997
8. W.C. Wake, Analysis of Rubbers and Rubber Like Polymers, 2ndEdn., Wiley-Interscience, 1969
9. ASTM standards for Rubber, Volume09.01
10. Bureau of Indian Standards for Latex, IS: 3708 (Part I) NRL-1 to10
11. Bureau of Indian Standards for Dry Rubber, IS: 3660 Part I, II and III

BMCP4P05: POLYMER CHARACTERIZATION PRACTICAL

Credit: 3 **Total Hours: 108**

Part I

Osmometry – determination of molecular weight of polymers by osmotic pressure method.

Viscometry – determination of molecular weight of polymers with dilute solution viscometry.

Part II

Estimation of monomers

Formaldehyde

MMA

Phenol

Part III

Systematic identification of virgin and compounded polymer sample:

Rubbers-NR, SBR, NBR, butyl rubber, neoprene, PB, polychloroprene

Plastics-PE, PP, PVC, nylon6, nylon 66, PVAl, PS, PMMA, ABS

Reference

1. J. Mitchell, Applied Polymer Analysis and Characterization, Hanser, 1992
2. H.H. Willard, L.L. Merrit, J.A. Dean, Instrumental Methods of Analysis, 3rdEdn., Van Nostrand,1963
3. G.C. Ives, J.A. Mead, M.M. Riley, Handbook of Plastics Test Methods, CRC Press, 1971
4. R.P. Brown, Handbook of Plastics Test Methods, 3rdEdn., Longman Scientific and Technical, 1988
5. Data Book on Plastics, Central Institute of Plastics Engineering and Technology, Madras
6. ASTM Standards for Rubber, Volume09.01

BMCP4P06: POLYMER PROCESSING AND TESTING PRACTICAL

Credit: 3 **Total Hours: 144**

1. Compounding and moulding-Plastics compounding, rubber compounding, latex compounding.
2. Cure characterization.
3. Polymer processing (extrusion, injection moulding, compression moulding, calendaring, thermoforming)
4. Composite preparation and characterization
5. Testing of mechanical properties of rubbers, plastics and composite (tensile, compression, shear, abrasion, tear, impact, hardness, flexural etc.)
   i. Stress – strain in tension, compression, flexure and shear
   ii. Tensile strength
   iii. Young's moduli
   iv. Tear strength
   v. Abrasion resistance
   vi. Flex resistance
   vii. Heat build up
   viii. Impact strength
   ix. Flexural tests
   x. Resilience
   xi. HDT
   xii. Hardness

Reference

1. R. P. Brown, Physical Testing of Rubber, 3rd Edn., Springer,1996
2. V. Shah, Handbook of Plastic Testing Technology, 2nd Edn, John Wiley & Sons, 1998
3. R. Brown, Handbook of Polymer Testing, Rapra Technology, 2002
4. R. P. Brown, Handbook of Plastics Test Methods, 3rd Edn., Longman Scientific and Technical, 1988
5. Data Book on Plastics, Central Institute of Plastics Engineering and Technology, Madras
6. ASTM standards for rubber, Volume 09.01

St Berchmans College

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