DEPARTMENT OF
CHEMISTRY

Curriculum and Syllabus for
Postgraduate Programme in
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 broad foundation in the latest developments in chemistry that enables scientific reasoning and analytical problem solving.
- To achieve the skills required in research and in chemical industry.
- To introduce modern instrumentation methods.
- To enhance the ability to communicate scientific information and research results to the society.
- Make the students capable to apply appropriate techniques for the qualitative and quantitative analysis of chemicals in laboratories and industries.
- To help in understanding the environmental issues.
- To Introduce the necessary skills for synthesise, separation and characterisation of compounds using laboratory and instrumentation techniques.

Programme Outcome

The programme will enable the students

- to interpret various issues related to scientific developments in terms of chemical terminology.
- to understand the experimental observations and prediction of outcomes.
- to handle modern instruments such as UV, IR, AAS......etc.
- to gain expertise in laboratory techniques.
- to gain expertise in appropriate techniques for the qualitative and quantitative analysis.

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 **Credit** 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 are 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

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.

<u>Model Mark cum Grade Card</u>

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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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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	BMCH101	Coordination Chemistry	4	72	4	25	75	100
	BMCH102	Mechanistic and Structural Organic Chemistry	4	72	4	25	75	100
	BMCH103	Classical and Statistical Thermodynamics	3	54	3	25	75	100
	BMCH104	Theoretical Chemistry	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 - I (P)	4	72				-
		Total	**25**	**450**	**15**	**100**	**300**	**400**
Semester II	BMCH205	Organometallics, Bioinorganic and Nuclear Chemistry	4	72	4	25	75	100
	BMCH206	Physical Organic Chemistry, Concerted Reactions and Reaction Intermediates	4	72	4	25	75	100
	BMCH207	Molecular Spectroscopy and Crystallography	4	72	4	25	75	100
	BMCH208	Advanced Quantum Mechanics and Chemical Bonding	3	54	3	25	75	100
	BMCH2P01	Inorganic Chemistry Practical – I (P)	3	54	3	25	75	100
	BMCH2P02	Organic Chemistry Practical - I (P)	3	54	3	25	75	100
	BMCH2P03	Physical Chemistry Practical - I (P)	4	72	3	25	75	100
		Total	**25**	**450**	**24**	**175**	**525**	**700**
Semester III	BMCH309	Solid State Chemistry and Inorganic Materials	4	72	4	25	75	100
	BMCH310	Synthetic Methods in Organic Chemistry	4	72	4	25	75	100
	BMCH311	Topics in Physical Chemistry	4	72	4	25	75	100
	BMCH312	Organic Spectroscopy	3	54	3	25	75	100
		Inorganic Chemistry Practical – II (P)	3	54	Evaluation at the end of fourth semester			-
		Organic Chemistry Practical - II (P)	3	54				-
		Physical Chemistry Practical – II (P)	4	72				-
		Total	**25**	**450**	**15**	**100**	**300**	**400**
Semester IV	BMCH413	Current Topics in Chemistry	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
	BMCH4P04	Inorganic Chemistry Practical - II (P)	3	54	3	25	75	100
	BMCH4P05	Organic Chemistry Practical - II (P)	3	54	3	25	75	100
	BMCH4P06	Physical Chemistry Practical - II (P)	4	72	3	25	75	100
	BMCH4PJ	Project	-	-	3	25	75	100
	BMCH4VV	Viva-Voce	-	-	2	-	100	100
		Total	**25**	**450**	**26**	**200**	**700**	**900**
			-	**-**	**80**	**575**	**1825**	**2400**

ELECTIVE COURSES

Course Code	Name of the Course
BMCH4E01	Advanced Inorganic Chemistry
BMCH4E02	Advanced Organic Chemistry
BMCH4E03	Advanced Physical Chemistry
BMCH4E04	Advanced Computational Chemistry

SEMESTER I

BMCH101: COORDINATION CHEMISTRY

Credit: 4 **Total Hours: 72**

Objectives

- To understand structural aspects and bonding in transition metal complexes
- To study in detail electronic spectra and magnetic properties of transition metal 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

After the successful completion of the course, the student shall acquire thorough knowledge on:

- Various aspects of structure and bonding in transition metal complexes
- Electronic spectra and magnetic properties of transition metal complexes
- 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: Structure and Bonding of Transition Metal 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 trigonal bipyramidal fields, LFSE, Dq values, Jahn-Teller (JT) effect, theoretical failure of crystal field theory, evidence of covalency in the metal-ligand bond, nephelauxetic effect, ligand field theory, molecular orbital theory-MO energy level diagrams for octahedral and tetrahedral complexes without and with π-bonding, experimental evidences for π -bonding.

Module 2: Spectral and Magnetic Properties of Transition Metal 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 & 2)

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 (Modules 1 & 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, 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 3: Kinetics and Mechanism of Reactions in Metal Complexes (18 hours)

3.1 Thermodynamic and kinetic stability, stepwise and overall formation constants, kinetics and mechanism of nucleophilic substitution reactions in square planar complexes, trans effect-theory and applications, trans influence.

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

3.3 Electron transfer reactions: outer sphere mechanism-Marcus theory, inner sphere mechanism-Taube mechanism.

Textbooks

1. B. E. Douglas, D. H. McDaniel, J. J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Edn., Wiley-India, 2007.
2. J. E. Huheey, E. A. Keiter, R. L. Keiter, O. K. Medhi, Inorganic Chemistry: Principles of Structure and Reactivity, 4th Edn., 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, 6th Edn., 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

Module 4: Stereochemistry of Coordination Compounds (9 hours)

4.1 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 catalyzed by coordination compounds.

4.2 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 5: Coordination Chemistry of Lanthanides and Actinides (9 hours)

5.1 General characteristics of lanthanides-Electronic configuration, Term symbols for lanthanide ions, Oxidation state, Lanthanide contraction. Factors that mitigate against the formation of lanthanide complexes. Electronic spectra and magnetic properties of lanthanide complexes. Lanthanide complexes as shift reagents.

5.2 General characteristics of actinides-difference between 4f and 5f orbitals, comparative account of coordination chemistry of lanthanides and actinides with special reference to electronic spectra and magnetic properties.

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

BMCH102: MECHANISTIC AND STRUCTURAL ORGANIC CHEMISTRY

Credit: 4 **Total Hours: 72**

Objectives

- To understand the various electronic factors deciding the molecular properties
- Study of mechanism of simple organic reactions
- Distinguish between aromatic and anti aromatic compounds.
- To familiarise the properties of aromatic and anti aromatic compounds.
- To gain a knowledge of symmetry properties of organic molecules.
- Differentiate chiral and achiral molecules.
- To learn various conformations of cyclic and acyclic compounds

Outcome

The course material will provide sufficient knowledge on:

- suitable mechanism of organic reactions
- Aromaticity of organic and the various reactions shown by aromatic compounds.
- Identify and draw structural isomers
- Identify the stereo enters in a molecule and assign the configuration.

Module 1: Organic Reaction Mechanism (18 hours)

1.1 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. Allylic strain Bonding weaker than covalent bonds - Hydrogen bonding and its effect of physical and chemical properties, Directional nature of hydrogen bond. Introduction to halogen bonding, carbon bonds and tetral bonds- three-centre-two-electron bond (3c–2e).

1.2 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.

1.3 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.

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

1.5 IUPAC nomenclature of spiro, bicycle, heterocyclic compounds, designation of organic reactions.

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, 2nd Edn. 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. P. Sykes, A Guidebook to Mechanism in Organic Chemistry, 6th Edn., Orient Longman Ltd., 1997
9. T. Okuyama, H. Maskill, Organic Chemistry: A Mechanistic Approach, Oxford University Press, 2014

Module 2: Aromaticity (18 hours)

2.1 Concept of aromaticity and anti-aromaticity: delocalization of electrons - 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 (18 hours)

3.1 Introduction to molecular symmetry and chirality with examples from common objects to molecules. 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 (atrop isomerism) 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, 4th Edn., 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. P. 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: Conformational Analysis (18 hours)

4.1 Conformational descriptors - factors affecting conformational stability of molecules-dipole interaction, bond opposition strain (torsional strain), bond angle strain and hydrogen bonding.

4.2 Conformational analysis of acyclic systems: ethane, substituted ethanes, dihalides, glycols, chlorohydrines etc., propane, *n*-butane, *n*-pentane, acetaldehyde, propionaldehyde and acetone.

4.3 Conformational analysis of cyclic systems: Conformations of carbocyclic rings from three to eight. Study of conformations of cyclohexane, mono, di and polysubstituted cyclohexanes, cyclohexanone (2-alkyl and 3-alkyl ketone effect), 2-halocyclohexanones (α-haloketone effect), cyclohexene and alkylidenecyclohexanes (allylic strains -$A^{1,2}$ and $A^{1,3}$). Anchoring group and conformationally biased molecules-their importance in assessing the reactivity of an axial or equatorial substituent. Conformation and anomeric effects in hexoses. Conformational structures of piperidine, N-Methylpiperidine. Conformational of fused and bridged bicyclic systems- decalins, adamantane, congressane and norborane.

4.4 Effect of conformation on the course and rate of elimination reactions in following acyclic systems:(i) Iodide catalysed debromination of *dl* and meso 2,3-dibromobutane and stilbene dibromide, (ii) Base catalysed dehydrohalogenation of (i) 2-bromobutane, (ii) *dl* and meso-stilbene dihalide (iii) erythro and threo- 1-bromo-1,2-diphenylpropane, (iii) pyrolytic elimination in *N,N*-dimethyl-s-butylamine oxide (Cope elimination). Chemical consequence of conformational equilibrium - Curtin Hammett principle.

4.5 Effect of conformation on reactivity of cyclohexane derivatives in the following reactions(steric assisted and steric hindered reactions): dehalogenation, dehydrohalogenation, semipinacolic deamination, pyrolytic elimination of esters (*cis*-elimination), nucleophilic substitution (S_N2, S_N1 and S_Ni) reactions, formation and cleavage of epoxides, esterification and hydrolysis, hydride reduction of cyclohexanones and oxidation of axial, equatorial cyclohexanols to cyclohexanone by chronic acid.

Textbooks

1. D. Nasipuri, Stereochemistry of Organic Compounds: Principles and Applications, 4^{th} Edn., New Academic Science Ltd., 2012
2. P. S. Kalsi, Stereochemistry Conformation and Mechanism, 8^{th} Edn., 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, 1^{st} Edn., RSC Tutorial Chemistry Text 1, 2001
3. T. Okuyama, H. Maskill, Organic Chemistry: A Mechanistic Approach, Oxford University Press, 2014

BMCH103: CLASSICAL AND STATISTICAL THERMODYNAMICS

Credit: 3 **Total Hours: 54**

Objectives

The course will enable the students to know

- Working knowledge of laws of thermodynamics
- Applying laws of thermodynamics to different systems.
- Particles and their distribution in various energy modes
- The correlation of bulk property to particle distribution
- The application of statistical methods for modelling

Outcome

The learners should be able to:

- Derive and interpret the laws of thermodynamics.
- understand the relationship between different thermodynamic functions at equilibrium conditions
- Explain the driving forces responsible for various changes
- Understand the statistical distribution of particles in different energy modes
- Calculate partition function and bulk properties
- Apply statistical mechanics for explaining the material properties

Module 1: Classical Thermodynamics (18 hours)

1.1 Entropy, dependence of entropy on variables of a system (S, T and V; S, T and P). Thermodynamic equations of state. Irreversible processes - Clausius inequality.

1.2 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, 6th Edn., 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, 6th Edn., McGraw Hill, 2009

Module 2: Thermodynamics of Irreversible Process and Bioenergetics (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, 6th Edn., Mc Millan Publishers, 2013

Reference

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

Module 3: Statistical Thermodynamics (18 hours)

3.1 Permutation, probability, 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. L. K. Nash, Elements of Statistical Thermodynamics, 2nd Edn., Dover Books, 2006

Module 4: Quantum Statistics (9 hours)

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

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, 2^{nd} Edn., New Age International, 2007
2. B. K. Agarwal, Statistical Mechanics, 2^{nd} 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. L. K. Nash, Elements of Statistical Thermodynamics, 2^{nd} Edn., Dover Books, 2006

BMCH104: THEORETICAL CHEMISTRY

Credit: 4 **Total Hours: 72**

Objectives

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

Outcome

1. Problem solving, critical thinking and analytical reasoning as applied to scientific problems.
2. Solve problems related to many electron systems
3. Find out the symmetry groups of molecules
4. Orthogonality theorem to molecules and to construction of character table.
5. Able to find out the allowed transitions in molecules using character table.

Module 1: Basics of Quantum Mechanics (12hours)

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

1.2 Atomic Orbitals: Hydrogen like, Slater and Gaussian type AOs, Plots and general features; Slater Determinants, examples and significance; Pauli's Exclusion Principle.

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, 2017

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, 3rd Edn 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 2: Applications of Quantum Mechanics to Simple Chemical Systems (24 hours)

2.1 Quantum mechanics of a free particle in motion; Particle on a ring: Circular Harmonics, Normalized wave functions, quantization of energy.

2.2 Particle in one dimensional box with infinite potential walls, normalized wave functions, calculation of energy; Particle in a 3D box: Calculation of Energy, Degeneracy; Quantum Mechanics of Harmonic Oscillator: Hermite, 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

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. V. 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, 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. R. 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. V. 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
11. Morgen & Murphey, Mathematics of Physics and Chemistry, An East-West edn 1964

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_3 using Cartesian coordinates and internal coordinate methods. Complementary character of IR and Raman spectra - determination of the number of active IR and Raman lines. Application in electronic spectra: selection rules for electronic transition, electronic transitions due to the carbonyl chromophore in formaldehyde.

Textbooks

1. K. V. 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

SEMESTER II

BMCH205: ORGANOMETALLICS, BIOINORGANIC AND NUCLEAR CHEMISTRY

Credit: 4 **Total Hours: 72**

Objectives

- to gain extensive knowledge about molecular organometallic chemistry
- to gain most important classes of ligands found in organometallic compounds
- to gain broad knowledge of nomenclature, coordination modes, geometries, and fundamental reaction types
- to gain knowledge of the chemical bonds and the theories that explain the electronic properties within organometallic compounds
- to gain knowledge on how to establish the relationship between the structures, chemical bonds in organometallic chemistry to determine and elucidate mechanisms in catalysis
- 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

The student shall able to get an idea about

- 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
- hypotheses and critically evaluate information from various sources related to organometallic chemistry and catalysis subjects
- the central content of the subject both in written and verbal form and by use of expressions characteristic for the subjects.

Module 1: Organometallic Compounds-Synthesis, Structure and Bonding (18 hours)

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

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

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

1.4 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, 5th Edn., Pearson, 2011
2. N. N. Greenwood, A. Earnshaw, Chemistry of the Elements, 2nd Edn., Butterworth Heinemann, 2004
3. B. E. Douglas, D. H. McDaniel, J. J. Alexander, Concepts and Models of Inorganic Chemistry, 3rdEdn., Wiley-India, 2007
4. P. Atkins, T. Overton, J. Rourke, M. Weller, F. Armstrong, Inorganic Chemistry, 5th Edn., Oxford University Press, 2010

Module 2: Reactions of Organometallic Compounds (9 hours)

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

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

2.3 Rearrangement reactions, redistribution reactions, fluxional isomerism.

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 3: Catalysis by Organometallic Compounds (9 hours)

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

3.2 Reactions of carbon monoxide and hydrogen-the water gas shift reaction, Fischer-Tropsch reaction (synthesis of gasoline), hydroformylation of olefins using cobalt or rhodium catalyst. Polymerization by organometallic initiators and templates for chain propagation-Ziegler Natta catalysts.

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

Textbooks

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. 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 4: Biocoordination Chemistry (18 hours)

4.1 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.

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

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

4.4 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.

4.5 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.

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

4.7 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.

4.8 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, Biocoordination Chemistry, Oxford Science Publication, 1995
2. T. Overton, J. Rourke, F. Armstrong, P. Atkins, M. Weller, Inorganic Chemistry, 5th Edn., 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, 4th Edn., 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 5: Nuclear Chemistry (18hours)

5.1 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

5.2 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.

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

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

5.5 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, 4th Edn., New Age International (P) Ltd., 2007
2. U. N. Dash, Nuclear Chemistry, 2nd Edn., 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, 1st Edn., John Wiley & Sons, 2006

2. G. Friedlander, J. W. Kennedy, E. S. Macias, J. M. Miller, Nuclear and Radiochemistry, 3rd Edn., John Wiley & Sons, New York, 1981
3. S. Glasstone, Sourcebook on Atomic Energy, 3rd Edn., Krieger Publishing Company, 1979

BMCH206: PHYSICAL ORGANIC CHEMISTRY, CONCERTED REACTIONS AND REACTION INTERMEDIATES

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

- Students can understand various physical and chemical factors controlling organic reactions.
- Enables the students to understand the underlying mechanism for all photochemical processes.
- The students can understand the importance of intermediate chemistry

Module 1: Physical Organic Chemistry (18 hours)

1.1 Energy Surfaces, reaction coordinates, transition states and intermediates, 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. 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.

1.2 Effect of structure on reactivity - quantitative treatment: Linear free energy relationship (LFER) in determination of organic reaction mechanism, The Hammett equation and its applications, interpretation of σ-values and reaction constants ρ. The Taft model, Solvent effects-Grunwald-Winstein plots and solvent polarity parameters.

1.3 Catalysis: General principles of catalysis, specific and general catalysis, nucleophilic catalysis and covalent catalysis. Importance of catalysis in the following reactions: (i) formation and cleavage of acetals (ii) formation of cyanohydrin, (iii) ester formation and hydrolysis reactions. Phase transfer catalysis and applications. Concept of hard and soft acids and bases- HSAB theory- Lewis acid-base interactions and relative nucleophilicity and electrophilicity.

Textbooks

1. E. V. Anslyn, D. A. Dougherty, Modern Physical Chemistry, University Science Books, 2005
2. R. H. Crabtree The Organometallic Chemistry of the Transition Metals, 5th Edition Wiley, 2009.

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 (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, 3rd Edn., 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, 1st Edn., 1971

Module 3: Carbocations, Carbanions and Enolates (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: Carbenes, Nitrenes, Free Radicals and Ylides (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

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. J. J. Li, Name Reactions: A Collection of Detailed Mechanisms and Synthetic Applications, 5th Edn., Springer Science & Business Media, 2014
3. P. Chaloner, Organic Chemistry: A Mechanistic Approach, CRC Press, 2014
4. L. Kuerti, B. Czako, Strategic Applications of Named Reactions in Organic Synthesis, Elsevier Academic Press, 2005.
5. M. B. Smith, Organic Synthesis, 3rd Edn., Wavefunctions Inc, 2011.
6. F. A. Carey, R. J. Sundberg, Advanced Organic Chemistry, Part A and B, 5th Edn., Springer, 2007

7. G. S. Zweifel, M. H. Nantz, Modern Organic Synthesis: An Introduction, 2nd Edn., John Wiley & Sons, 2017
8. P. Wyatt, Stuart Warren, Organic Synthesis Strategy and Control, John Wiley & Sons, 2013

BMCH207: MOLECULAR SPECTROSCOPY AND CRYSTALLOGRAPHY

Credit: 4 **Total Hours: 72**

Objectives

The major objectives are

- To study theory of interaction of light and matter
- to understand various energy levels of molecules/particles
- Elucidate the structure from spectral data
- The basic instrumentation of various spectroscopic methods

Outcome

The students shall be able to

- Understand the interaction of various components of EM radiation with matter
- Calculate the energy levels, internuclear distance etc.
- To predict the structure/spectrum of molecules

Module 1: Foundations of Spectroscopic Techniques (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, 5^{th} Edn., 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 Atta-ur-Rahman, NMR Spectroscopy, Wiley, 1995
3. , 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 (27 hours)

2.1 NMR spectroscopy: magnetic properties of nuclei, 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, 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, magic angle spinning.

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, 5th Edn., 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: Crystallography (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. C. Giacovazzo, Fundamentals of Crystallography, 3rd Edn., Oxford Science Publications, 2002
2. P. J. Collings, M. Hird, Introduction to Liquid Crystals: Chemistry and Physics, 1st Edn., Taylor & Francis, 1997

Reference

1. D. 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, P. Sheng, E. B. Priestley, Introduction to Liquid Crystals, Springer, 1974

BMCH208: ADVANCED QUANTUM MECHANICS AND CHEMICAL BONDING

Credit: 3 **Total Hours: 54**

Objectives

1. To familiarize the theoretical concepts of many electron systems.
2. To understand the importance of approximation methods in theoretical Chemistry
3. To familiarize the chemical aspects of boning

Outcome

1. Knowledge of higher level theoretical concepts
2. Ability to understand molecular reactivity based on chemical bonding
3. Able to solve problems related to many electron systems

Module 1: Approximation Methods (18 hours)

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

1.2 Variation Method: Variation theorem and proof, Rayleigh Ratio, Rayleigh-Ritz Method, Illustration with simple trial functions, Application of Variation theorem to Helium atom, Calculation of ground state energy, Comparison with experimental value.

1.3 Perturbation Method: General Concept, Time-independent perturbation method, non-degenerate case, first-order correction to energy and wave functions with derivations; Examples: Helium atom, Particle in a 1D box with slanted bottom, anharmonic oscillator.

1.4 Self-Consistent Field Methods: General Concepts and Algorithm for HSCF method, Concept of Basis functions, Roothan-Hall equations, Hartree-Fock Self consistent field method: Algorithm.

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 2: Chemical Bonding (27 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 4: Applications of Group Theory in Chemical Bonding (9 hours)

4.1 Application in quantum mechanics, transition moment integral, vanishing of integrals. Applications in chemical bonding, construction of hybrid orbitals with BF_3, CH_4, PCl_5, XeF_4as examples. Transformation properties of atomic orbitals. Symmetry adapted linear combinations (SALC) of C_{2v}, C_{2h}, C_3, C_{3v} and D_{3h}. Jahn-Teller effect. Woodward Hoffmann rules-correlation diagram.

Textbooks

1. K. V. Reddy, Symmetry and Spectroscopy of Molecules, New Age Science Ltd; 2nd Edn., 2009
2. S. Swarnalakshmi, T. Saroja, R.M. Ezhilarasi, A Simple Approach to Group Theory in Chemistry, Universities Press, 2008
3. V. Ramakrishnan, M.S. Gopinathan, Group Theory in Chemistry, Vishal Publications, 2nd Reprint edition 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. Agarwal, Molecular Symmetry in Chemistry *via* Group Theory, Ane Books Pvt. Ltd, 2013
6. R. L. Carter, Molecular Symmetry and Group Theory, John Wiley & Sons, 1997
7. Bhagi& Jain Raj, Group Theory & Symmetry in Chemistry, Krishna Prakashan Media (P) Ltd, 2014
8. H. H. Jaffe, M. Orchin, Symmetry in Chemistry, Dover Publications Inc., 2003
9. D. 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, 2000
11. A.S. Kunju, G. Krishnan, Group Theory and its Applications in Chemistry, PHI Learning, 2nd edition (2010)

SEMESTERS I AND II

PRACTICAL

BMCH2P01: 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

BMCH2P02: 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, 4th Edn., 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

BMCH2P03: 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. Thermochemistry experiments

1. Determination of heat of neutralization of strong acid and strong base.
2. Determination of strength of the given strong acid.

III. 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

IV. 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).

V. 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

BMCH309: SOLID STATE CHEMISTRY AND INORGANIC MATERIALS

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: Solid State Chemistry (18 hours)

1.1 Structure of solids: types of close packing - hcp and ccp, packing efficiency, radius ratios, structure types - NaCl, Na_2O, $CdCl_2$,CdI_2 zinc blende, wurtzite, nickel arsenide, fluorite and antifluorite, CsCl, rutile and Cs_2O, perovskite, ABO_3, K_2NiF_4, spinels and inverse spinels.

1.2 Imperfections in solids-point defects-colour centres, line defects and plane defects.

1.3 Solid state reactions-diffusion coefficient, mechanisms, vacancy diffusion, thermal decomposition of solids-Type I reactions, Type II reactions.

1.4 Phase transition in solids: classification of phase transitions-first and second order phase transitions, kinetics of phase transitions, Martensitic transformations, order-disorder transitions and spinodal decomposition, sintering.

1.5 Methods of Single Crystal Growth: Solution growth; Melt Growth-Bridgeman, Czochralski, Kyropoulus, Verneuil; Chemical Vapour Transport; Fused Salt Electrolysis; Hydrothermal method; Flux Growth.

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

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

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

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

2.4 Super conductivity-Type I and Type II superconductors, Cooper pairs, theory of low temperature super conductors, Josephson effect- junctions using superconductors, BCS theory of superconductivity (derivation not required). Super conducting cuprates-YBaCu oxide system, Meissner effect, conventional superconductors, organic superconductors, fullerenes abd carbon nanotubes as superconductors, high temperature superconductors.

Textbooks (Modules 1 and 2)

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 (Modules 1 and 2)

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 3: Inorganic Chains and Rings (18 hours)

3.1 Catenation, heterocatenation.

3.2 Silicate minerals - Structure of silicates - common silicates, silicates containing discrete anions, silicates containing infinite chains, silicates containing sheets, framework silicates. Zeolites-synthesis, structure and applications. Silicones – synthesis, structure and applications.

3.3 Isopoly acids of vanadium, molybdenum and tungsten. Heteropoly acids of Mo and W. Condensed phosphates-preparation, structure and applications.

3.4 Polythiazil-one dimensional conductors.

3.5 Structure and bonding in borazines, phosphorous-nitrogen compounds - phosphazenes. Heterocyclic inorganic ring systems-structure and bonding in phosphorous-sulphur and sulphur-nitrogen compounds. Homocyclic inorganic ring systems-structure and bonding in sulphur, selenium and phosphorous compounds.

Textbooks

1. J. E. Huheey, E. A. Keiter, R. A. Keiter, Inorganic Chemistry Principles of Structure and Reactivity, 4th Edn., Pearson Education India, 2006.
2. B. R. Puri, L. R. Sharma, K. C. Kalia, Principles of Inorganic Chemistry, Vishal Publishing Co., 2017

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

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

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

4.2 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 anions 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 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

BMCH310: SYNTHETIC METHODS IN ORGANIC CHEMISTRY

Credit: 4 **Total Hours: 72**

Objectives

- To study different oxidation and reduction methods
- Understand the basics of asymmetric synthetis, photochemistry and supramolecular chemistry
- To design several metal mediated organic synthesis

Outcome

After the successful completion of the course, the students shall

- be familiar with cation, anion, radical, pericyclic and organometallic mediated processes
- analyze fundamental organic reactions and further transformations
- gain new insights into the factors governing the mechanistic, stereochemical and regiochemical course of reactions

Module-1 Oxidation and Reduction Methods (18 hours)

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

a. alcohols to carbonyls using Chromium, DMSO, TEMPO based reagents, Jones,
b. Collins-Ratcliff reagents, PCC, PDC, Swern oxidation, Dess - Martin Periodinane oxidation - DMP, tetrapropylammonium perruthenate - TPAP.
a. phenols (Fremy's salt, silver carbonate on Celite (Fetizon's reagent))
b. alkenes to epoxides (peracids based epoxidation – with special reference to peracid reactivity, stereoselectivity and chemoselectivity)
c. alkenes to diols: Prevost and Woodward hydroxylation
d. alkenes to carbonyls with bond cleavage: Ozonolysis
e. alkenes to alcohols/carbonyls without bond cleavage (hydroboration-oxidation, Wacker oxidation, Selenium based oxidation)
f. 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: Protecting Functional Groups and Reagents (9 hours)

2.1 Protection and deprotection of double and triple bonds, amino, carboxylic acid, carbonyl and hydroxyl groups, SSPS.

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

Textbooks

1. J. 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: Organic Photochemistry (9 hours)

3.1 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.

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

3.3 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.

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 4: Organometallic Reagents in Organic Synthesis (18 hours)

4.1 Use of organolithium agents: Preparation, reactivity, lithium halogen exchange, transmetalation, metallation, chemoselectivity, benzilic and allylic metallation, metallation 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.

Textbook

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

Reference

1. G. S. Zweifel, M. H Nantz, Modern Organic Synthesis: An Introduction, 2^{nd} Edn., John Wiley & Sons, 2017
2. P. Wyatt, S. Warren, Organic Synthesis Strategy and Control, John Wiley & Sons, 2013

Module 5: Supramolecular Chemistry (9 hours)

5.1 Concept of molecular recognition, host-guest complex formation clathrates and cavitands; podands, corands and cryptands forces involved in molecular recognition- spatial relationship.

5.2 Molecular receptors (gross structural features only; synthesis not expected): cyclodextrins, crown ethers, cryptands, spherands, tweezers, carcerands, cyclophanes, calixarenes, catenanes and olympiadanes.

5.3 Importance of molecular recognition in biological systems like DNA and protein. Protein biosynthesis- detailed study- codon and anticodon sensing, DNA sequencing and PCR-basics.

Textbooks

1. J. M. Lehn, Supramolecular Chemistry: Concepts and Perspectives, VCH, 1995
2. J. W. Steed, Jerry L. Atwood, Supramolecular Chemistry, 2nd Edn, John Wiley & Sons, 2009

Reference

1. F. Vogtle, Supramolecular Chemistry: An Introduction, Wiley, 1993

Module 6: Principles of Asymmetric Synthesis (9 hours)

6.1 Basic principles of Asymmetric synthesis: Introduction to asymmetric synthesis-importance of asymmetric synthesis, conditions for an efficient asymmetric synthesis-transition state criteria, energetic considerations,kinetic and thermodynamic control, double stereo differentiation- matched pair and mismatched pair.

6.2 Strategies for asymmetric synthesis- advantages and limitations of each strategy (basic idea only).

6.3 Analytical methods for determining enantiomeric excess: specific rotation, chiral NMR, chiral derivatizing agents, chiral solvent, chiral shift reagents and chiral HPLC.

6.4 Resolution: Racemic modification and resolution of racemic mixture. Resolving agents and resolution of racemic compounds having common functional groups for eg. alcohol, amine, acid. Kinetic resolution and dynamic kinetic resolution of racemic mixtures.

6.5 Introduction to the Chiral pool strategy: importance and applications.

Text Books

1. L. Poppe, M. Nógrádi, Stereochemistry and Stereoselective Synthesis: An Introduction, Wiley-VCH, 2016
2. R. E. Gawley, J. Aube, Principles of Asymmetric Synthesis, 2nd Edn., Elsevier Ltd., 2012

Reference

1. D. Nasipuri, Stereochemistry of Organic Compounds: Principles and Applications, 4th Edn., New Academic Science Ltd., 2012
2. E. L. Eliel, S. H. Wilen, Stereochemistry of Organic Compounds, John Wiley & Sons, New York, 2008
3. J. D. Morrison, *Asymmetric Synthesis: Vol 1: Analytical Methods*, 1st Edn., Academic Press, **1983**
4. P. Schreier, A. Bernreuther, M. Huffer, Analysis of Chiral Organic Molecules Methodology and Applications, Walter de Gruyter & Co., 1995

5. K. W. Busch, M. A. Busch, Chiral Analysis, 1st Edn., Elsevier, 2006

BMCH311: TOPICS IN PHYSICAL CHEMISTRY

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.

1.2 Theories of unimolecular reactions: Lindeman theory (derivation) – Modification of Lindeman theory -Hinshelwood theory (mechanism and qualitative idea), 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 Fast reactions: Relaxation technique, flow method, shock methods, flash photolysis, NMR technique and ESR methods of studying fast reactions.

1.5 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).

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

1.7 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, 3rd Edn., 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: Surface Chemistry (27 hours)

2.1 Different types of surfaces, thermodynamics of surfaces, Gibbs adsorption equation and its verification, surfactants and micelles, surface films, surface pressure and surface potential and their measurements and interpretation.

2.2 Adsorption: The Langmuir theory, kinetic and statistical derivation, multilayer adsorption-BET theory, Use of Langmuir and BET isotherms for surface area determination. Application of Langmuir adsorption isotherm in surface catalysed reactions, Eley-Rideal mechanism and Langmuir-Hinshelwood mechanism, flash desorption.

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

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

2.5 Application of low energy electron diffraction and photoelectron spectroscopy, ESCA and Auger electron spectroscopy, scanning probe microscopy, ion scattering, SEM and TEM in the study of surfaces.

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

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

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, 6th Edn., 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, 2nd Edn., Oxford University Press, 2011

Module 3: Photochemistry (18 hours)

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

3.2 Kinetics of photochemical processes, Stern – Volmer equation. Dimerization of anthracene, ozone layer in the stratosphere.

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

3.4 Solar energy utilization and storage, solar cell and its working, photochemistry of environment, greenhouse effect, photochemistry of vision and nucleic acids, 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-Mukherjee, Fundamentals of Photochemistry, 3rd Edn., 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

Module 4: Introduction to Electrochemistry (9 hours)

4.1 Theories of ions in solution, Drude and Nernst's electrostriction model and Born's model, Debye-Huckel theory, Derivation of Debye-Huckel-Onsager equation, validity of DHO equation for aqueous and non-aqueous solutions, Debye- Falkenhagen effect, conductance with high potential gradients.

4.3 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.

Textbook

1. 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
2. D. R. Crow, Principles and Applications of Electrochemistry, 4th Edn., S.Thornes, 1994

BMCH312: ORGANIC SPECTROSCOPY

Credit: 3 **Total Hours: 54**

Objectives

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

- Predict the structure 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 (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: Nuclear Magnetic Resonance Spectroscopy (18 hours)

3.1 Magnetic nuclei with special reference to ^{1}H and ^{13}C nuclei. Chemical shift and shielding/deshielding, factors affecting chemical shift, relaxation processes, chemical and magnetic non-equivalence, local diamagnetic shielding and magnetic anisotropy. ^{1}H and ^{13}C NMR scales.

3.2 Spin-spin splitting: AX, 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 of 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 MRI.

3.6 Problems on spectral interpretation with examples.

Module 4: Mass Spectrometry (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

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

Reference

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. A.U. Rahman, M.I. Choudhary, Solving Problems with NMR Spectroscopy, Academic Press, 1996.
6. L. D. Field, S. Sternhell, J. R. Kalman, Organic Structures from Spectra, 4th Edn., John Wiley & sons, 2007.
7. C.N. Banwell, E.M. McCash, Fundamentals of Molecular Spectroscopy, 4th Edn., Tata McGraw Hill, 1994.
8. D.F. Taber, Organic Spectroscopic Structure Determination: A Problem Based Learning Approach, Oxford University Press, 2007.
9. F. Bernath, Spectra of Atoms and Molecules, 2nd Edn., Oxford University Press, 2005.
10. E.B. Wilson Jr., J.C. Decius, P.C. Cross, Molecular Vibrations: The Theory of Infrared and Raman Vibrational Spectra, Dover Pub., 1980.

SEMESTER IV

BMCH413: CURRENT TOPICS IN CHEMISTRY

Credit: 3 **Contact hours: 54**

Objectives

The main objectives of this paper is to

- Introduce students into the world of nanomaterials
- To make them aware of the new strategies in organic synthesis and asymmetric synthesis
- Introduce various scientific research methods

Outcome

- To be aware of the applications of various nanomaterial
- Be able to design the total synthesis of a compound
- Read and write a scientific article

Module 1: Nanomaterials (18 hours)

1.1 One dimensional, two dimensional and three dimensional nanostructured materials, size dependent properties – quantum confinement – optical properties - specific heat and melting point- mechanical properties – super plasticity - plastic deformation of ceramics - nanoceramics - catalytic properties, Moore's law.

1.2 Synthesis and properties of fullerenes, comparison of structure of $C_{60}$and C_{70}, carbon nanotubes – arc discharge method, catalytic chemical vapour deposition, electric arc method, properties, metal nanoparticles – synthesis of nanoparticles of gold and silver, self-assembled monolayers - preparation, growth process and applications.

1.3 Gas phase clusters – laser vapourisation, pulsed arc cluster ion source, supersonic nozzle sources, Wien filter, Quadrupole mass filter and time of flight mass filter. Quantum dots – synthesis in confined media, molecular precursor route, applications

1.4 Nanoshells-types of systems and applications.

1.5 Application of nanoscience – nanosensors – preparation, nanomedicines – various nanosystems and applications.

Textbooks

1. T. Pradeep, Nano the Essentials, Understanding Nanoscience and Nanotechnology, McGraw Hill, 2008

2. G. Cao, Nanostructures & Nanomaterials-Synthesis, Properties and Applications, Imperial College Press, 2004
3. G. Schmidt, Nanoparticles: From theory to Applications, Wiley, 2004

Reference

1. C. N. R. Rao, A. Muller, A. K. Cheetham (Eds.), The Chemistry of Nanomaterials: Synthesis, Properties and Applications, Wiley, 2004
2. B. Bhushan (Ed.), Handbook of Nanotechnology, 3rd Edn, Springer-Verlag, 2010
3. C. N. R. Rao, A. Muller, A. K. Cheetham, Eds., Nanomaterials Chemistry – Recent Developments and New Directions, Wiley-VCH, 2007

Module 2: New Synthetic Strategies in Organic Chemistry (9 hours)

2.1 Tandem, domino, multicomponent, remote functionalization reactions. One pot synthesis, Green organic synthesis- twelve principles of green chemistry, microwave assisted synthesis, ultra sound assisted synthesis. Click reactions, Combinatorial Synthesis. Linear and convergent synthesis, Electro organic synthesis, Enzyme catalysed organic reactions.

2.2 Synthesis of metallocenes, non-benzenoid aromatics and polycyclic aromatic compounds. Organic chemistry research developments during last ten years.

Textbook

1. J. Singh, L. D. S. Yadav, Organic Synthesis, Pragtahi Prakashan, 2014

Reference

1. M. B. Smith, March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure, 7th Edn., Wiley, 2015
2. C. K. Charles, Organic Synthesis, Narosa Publishers, 2012
3. J. M. Coxon, R. O. C. Norman, Principles of Organic Synthesis, 2nd Edn., Springer, 2012

Module 3: Methodologies in Asymmetric Synthesis (18 hours)

3.1 Chiral Substrate controlled asymmetric synthesis: Nucleophilic additions to α–chiral carbonyl compounds. 1, 2- asymmetric induction-Prediction of stereochemistry by Cram’s rule, Felkin-Anh model and Cram’s chelate model. Diastereoselective aldol reactions (chiral enolate-achiral aldehydes and achiral enolate-chiral aldehydes)- explanation by Zimmerman-Traxel model.

3.2 Chiral auxiliary controlled asymmetric synthesis: Evan’s enantioselective enolate α-alkylation, Enders SAMP/RAMP hydrazone alkylation, Asymmetric Diels-Alder cycloaddition reactions with chiral*α,β*-unsaturated *N*-acyloxazolidinones, Evan's asymmetric*syn*aldol reaction.

3.3 Chiral reagent controlled asymmetric synthesis: BINAL-H and CBS reagents for asymmetric reductions of prochiral ketones, Asymmetric hydroboration using Ipc_2BH and $IpcBH_2$

3.4 Chiral catalyst controlled asymmetric synthesis: Sharpless asymmetric epoxidation (SAE), asymmetric dihydroxylation (SAD) and asymmetric aminohydroxylation (SAA), Jacobsen's asymmetric epoxidation, Noyori asymmetric hydrogenation of functionalized olefins and ketones.

3.4.1 Asymmetric organocatalysis: Proline catalysed aldol reactions, Intramolecular Michael addition reaction by Imidazolidinone (Macmillan) catalysts, Shi epoxidation, (Thio)-urea catalyzed enantioselective addition to imines (Strecker Reaction).

3.4.2 Enzyme mediated asymmetric catalysis (asymmetric biocatalysis): Enzyme classes and related chemical reactions (basic idea only), advantages and disadvantages of biocatalysis.

Text Books

1. H. B. Kagan, Asymmetric Synthesis, Ist Edn., Thieme Medical Publishers, 2003
2. L. Poppe, M. Nógrádi, Stereochemistry and Stereoselective Synthesis: An Introduction, Wiley-VCH Verlag GmbH & Co., 2016
3. R. E. Gawley, J. Aube, Principles of Asymmetric Synthesis, 2nd Edition, Elsevier Ltd., 2012

Reference

1. J. D. Morrison, Asymmetric Synthesis: Vol 1- 5, 1st Edn., Academic Press, 1983
2. V. Caprio, J. M. J. Williams, Catalysis in Asymmetric Synthesis, 2nd Edn., John Wiley and Sons, Ltd., 2009
3. I. Ojima, Catalytic Asymmetric Synthesis, 3rd Edition, John Wiley & Sons, Inc., 2010
4. E. N. Jacobsen, P. A. Yamamoto, H. Yamamoto, Comprehensive Asymmetric Catalysis, Springer 2000
5. R. Noyori, Asymmetric Catalysis in Organic Synthesis, John Wiley & Sons, 1994
6. A. Berkessel, H. Groeger, Asymmetric Organocatalysis, Wiley-VCH, 2005
7. A. Patti, Green Approaches to Asymmetric Catalytic Synthesis, Springer, 2011
8. G. Grogan, Practical Biotransformations: A Beginner's Guide, John Wiley and Sons, Ltd., 2009

Module 4: Scientific Research Methods (9 hours)

4.1 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. Important journals in Chemistry.

4.2 Scientific Writing: Structure of Research paper, thesis and books. Journal articles, communications, reviews etc. Referencing styles. Art of writing research paper Plagiarism. Peer review process, Introduction to reference management softwares. Practical use of Mendeley software.

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. J. 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**)**

BMCH4E01: ADVANCED INORGANIC CHEMISTRY

Credit: 3 **Total Hours: 72**

Objectives:

- To study in detail the applications of group theory in inorganic chemistry.
- To elucidate spectra of complexes using character table.
- To understand the construction of energy level diagrams in coordination chemistry by group theoretical considerations.
- To learn inorganic spectroscopic methods.
- To study in detail the basics of inorganic photochemistry.
- To understand various analytical methods
- To learn the chemistry of acids and bases and non-aqueous solvents.

Outcome

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

- to elucidate spectra of complexes using character table
- inorganic spectroscopic methods
- basics of inorganic photochemistry
- various analytical methods
- chemistry of acids and bases and non-aqueous solvents

Module 1: Applications of Group Theory (27 hours)

1.1 Transformation properties of atomic orbitals, hybridization schemes for sigma and pi bonding with examples, Symmetry Adapted Linear Combination of Atomic orbitals in tetrahedral, octahedral and sandwich complexes.

1.2 Ligand field theory-splitting of d orbitals in different environments using group theoretical considerations, construction of energy level diagrams, correlation diagrams, method of descending symmetry, formation of symmetry adapted group of ligands, MO diagrams, splitting terms for orbitals, energy levels, d-d transition-selection rules, vanishing integrals. Raman spectra of complexes with oxo anions as ligands, IR and Raman spectra using character tables in tetrahedral, octahedral and square planar complexes.

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 2: Inorganic Spectroscopic Methods (9 hours)

2.1 Infrared and Raman Spectroscopy: structural elucidation of coordination compounds containing the following molecules/ions as ligands - NH_3, H_2O, CO,NO, OH^-, SO_4^{2-}, CN^-, SCN^-, NO_2^- and X^- (X=halogen).

2.2 Electron Paramagnetic Resonance Spectroscopy: EPR of d^1 and d^9 transition metal ions in cubic and tetragonal ligand fields, evaluation of g values and metal hyperfine coupling constants.

2.3 Mössbauer Spectroscopy: applications of Mössbauer spectroscopy in the study of Fe(III) complexes.

Textbook

1. K. Nakamoto, IR and Raman Spectra of Inorganic and Coordination Complexes, Part A-Theory and Applications in Inorganic Chemistry, 6th Edn., John Wiley &Sons, 1997

Reference

1. R. S. Drago, Physical Methods in Chemistry, Saunders College, 1992

Module 3: Inorganic Photochemistry (9 hours)

3.1 Excited states, ligand field states, charge-transfer states and Thexi states, phosphorescence and fluorescence. Photochemical reactions-substitution and redox reactions of Cr(III), Ru(II) and Ru(III) complexes. Applications-synthesis and catalysis, chemical actinometry and photochromism. Metal-metal multiple bonds.

3.2 Metal complex sensitizers-electron relay, semiconductor supported metal oxide systems, water photolysis, nitrogen fixation and 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 4: Analytical Methods (18 hours)

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

4.2 Decompositions and dissolution-reagents for decomposition and dissolution like HCl, H_2SO_4, HNO_3, $HClO_4$ and HF. Microwave decompositions, combustion methods. Uses of fluxes like Na_2CO_3, Na_2O_2, KNO_3, $K_2S_2O_7$, NaOH, B_2O_3 and lithium meta borate.

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

4.4 Analytical procedures involved in the environmental monitoring of water quality-BOD, COD, DO, nitrite and nitrate, iron, fluoride, soil moisture, salinity, soil colloids, cation and anion exchange capacity. Air pollution monitoring: sampling and collection of air pollutants-SO_2, NO_2, NH_3, O_3, and SPM.

Textbooks

1. D.A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, Fundamentals of Analytical Chemistry, 8th Edn., Saunders College, 2007
2. J.G. Dick, Analytical chemistry, McGraw-Hill, 1973

Reference

1. S. E. Manahan, Environmental Chemistry, 9th Edn., CRC Press, 2010
2. J. E. Huheey, E. A. Keiter, R. L. Keiter, O. K. Medhi, Inorganic Chemistry: Principles of Structure and Reactivity, 4th Edn., Pearson Education, 2006
3. H .J. Emeleus, A. G. Sharpe, Modern Aspects of Inorganic Chemistry, 4th Edn., ELBS, 1973
4. K. F. Purcell, J. C. Kotz, Inorganic Chemistry, Holt-Saunders, 1977

Module 5: Acids and Bases and Non-aqueous Solvents (9 hours)

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

5.2 Reactions in non-aqueous solvents. Ammonia - solutions of metals in liquid ammonia. Protonic solvents: anhydrous sulfuric acid, hydrogen halides. Aprotic solvents: non-polar solvents, non-ionizable polar solvents, polar solvents undergoing autoionization, liquid halogens, inter-halogen compounds, oxy halides, dinitrogen tetroxide, sulphur dioxide.

Textbooks

1. B. R. Puri, L. R. Sharma, K. C. Kalia, Principles of Inorganic Chemistry, Vishal Publishing Co., 2017
2. J. D. Lee, Concise Inorganic Chemistry, 5^{th} Edn., Wiley India (P) Ltd., 2010

Reference

1. J. E. Huheey, E. A. Keiter, R. L. Keiter, O. K. Medhi, Inorganic Chemistry: Principles of Structure and Reactivity, 4^{th} Edn., Pearson Education, 2006
2. F. A. Cotton, G. Wilkinson, C. A. Murillo, M. Bochmann, Advanced Inorganic Chemistry, 6^{th} Edn., John Wiley & Sons Inc., 1999

BMCH4E02: ADVANCED ORGANIC CHEMISTRY

Credit: 3 **Total Hours: 72**

The main objectives of this course are

- To introduce the students to the advanced organic reactions and organic polymers
- To understand the basic concepts of retrosynthetic analysis and apply it to the synthesis of natural products
- To introduce the basics of medicinal chemistry and construction of carbocyclic rings and natural products

Outcome

- Will study the mechanism and applications of several organic reactions
- Will learn to design the synthesis of a compound using retrosynthetic tools
- Understand the basics of medicinal and polymer chemistry
- Will study different natural products

Module 1: Important Organic Reactions (9 hours)

1.1 Shapiro reaction, Julia elimination, Rupe rearrangement and Benzilic acid rearrangement, Prins reaction. Sommelet-Hauser, Favorskii, Schmidt, Neber, Bayer -Villiger, Benzidine, Stevens and Wittig rearrangements. Baylis Hilman reaction, Ritter reaction and Brook rearrangement, Benzoin condensation. Seyferth-Gilbert homologation.

1.2 Extrusion reactions- Storey synthesis, azo, S, CO_2, CO extrusion reactions. Dyotropic rearrangements, Noncyclic rearrangement, Chapman rearrangement, Wallach rearrangement,

Textbook

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

Reference

1. M. B. Smith, March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure, 7th Edn., Wiley, 2015
2. S. Delvin, Organic Reagents and Name Reactions, Sarup and Sons, 2011

Module 2: Retro Synthetic Analysis (18 hours)

2.1 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 (Retrosynthesis of at least 40 compounds).

2.2 Retro and forward synthesis of nuciferal, Corey lactone, luciferin and juvabione, Reserpine and longifolene.

Textbook

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

Reference

1. R. K. 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

Module 3: Medicinal Chemistry (9 hours)

3.1 Development of a drug, Drugs, theories of drug action like drug-receptor theory, occupancy theory, induced fit theory, activation- Steps of drug action (selectivity, administration, absorption, binding, excretion etc.). LD50, ED50, therapeutic index, agonist and antagonists. Drug SAR and QSAR with two examples.

3.2 Important chemicals used in drug action-, antipyretics, antimalarial drugs, anti HIV drugs and anticancer drugs. Central nervous system acting drugs

Antibiotics - sulpha drugs, classical and modern antibiotics like penicillin, chloramphenicol, tetracycline, streptomycin, cephalosporins – structure and uses.

(Synthesis of drugs not expected).

Textbooks

1. Ashutosh Kar, Medicinal Chemistry, 5th Edition, New Age International Publishers, 2010
2. D. Sriram, P. Yogeeswari, Medicinal Chemistry, 2nd Edition, Pearson, 2010

Reference

1. G. Patrick, An Introduction to Medicinal Chemistry, 5th Edition, Oxford University Press, 2013
2. D. J. Abraham (Editor), David P. Rotella, Burger's Medicinal Chemistry, Drug Discovery, and Development, 7th Edition, John Wiley and Sons, 2010
3. J. H. Block, John M. Beale, Jr., Wilson & Gisvold's Textbook of Organic Medicinal and Pharmaceutical Chemistry, 12th Ed, Lippincott Williams & Wilkins, 2011

4. L. M. Atherden, Bentley and Drivers Textbook of Pharmaceutical Chemistry, Oxford University Press, 2010

Module 4: Natural Products (18 hours)

4.1 Classification and Nomenclature of prostaglandins (Structural elucidation not expected). Forward synthesis of prostaglandins PGE_2 and $PGF_{2\alpha}$.

4.2 Carbohydrates- Disaccharides- sucrose, lactose and maltose- structure and conformation, Structure of starch and cellulose.

4.3 Proteins and nucleic acids. Structure of proteins, DNA and RNA, Replication of DNA, protein biosynthesis, transcription and translation.

4.4 Terpenoids, alkaloids, anthocyanins, flavonoids, vitamins and Steroids: Introduction, classification and properties.

4.5 Forward synthesis of 11α-hydroxyprogesterone, testosterone, Inter-conversions of steroids, camphor, atropine, papaverine, quinine, cyanin, quercetin, β-carotene, Vitamin D.

4.6 Biosynthesis: Basic principles of the biosynthesis of terpenes, steroids, alkaloids, carbohydrates, proteins and nucleic acids. Biosynthesis of cholesterol, morphine and phenylalanine. Biomimetic synthesis of progesterone and spatreine.

Textbooks

1. I. L. Finar Organic Chemistry, Vol. 1, 6th Edition, Pearson, 2002
2. I. L. Finar Organic Chemistry, Vol. 2, 6th Edition, Pearson, 2002
3. S. V. Bhat, B. A. Nagasampaki, M. Sivakumar, Chemistry of Natural Products, Narosa Publications, 2005

Reference

1. D. Voet, J. G. Voet, Biochemistry, Wiley, 2ndEdn., 1995
2. J. Mann, Chemical Aspects of Biosynthesis, Oxford Chemistry Primer No. 20, 1994
3. E. Poupon, Bastien Nay (Eds.), Biomimetic Organic Synthesis, 1stEdn., Wiley-VCH, 2011

Module 5: Organic Polymers (9 hours)

5.1 Classification of polymers, Types of polymerization – addition, free radical, ionic and coordination polymerization – Zeigler-Natta, condensation polymerization – Mechanism.

5.2 Organic polymers - polyethylene, polypropylene, polyvinyl chloride, polyamides, polyesters, phenolic resins, epoxy resins, natural and synthetic rubbers.

5.3 Dendrimers – Types and applications, hyper branched polymers.

5.4 Biodegradable polymers, liquid crystal polymers, fire retardant polymers. Polymer supported reagents- Merrifield resins and applications.

Textbooks

1. Fritz Vögtle, Gabriele Richardt, Nicole Werner, Dendrimer Chemistry, Wiley-VCH, 2009
2. Charles E. Carraher, Polymer Chemistry, 6^{th} Edn., Marcel Dekker, 2003
3. K. J. Saunders, Organic Polymer Chemistry, 2^{nd} Edn., Chapman and Hall, 1988
4. R.W. Dyson, Speciality Polymers, Chapman and Hall, 1987

Reference

1. W. T. Ford, Polymeric Reagents and Catalysts An Overview, ACS Symposium Series, American Chemical Society,1986

Module 6: Synthesis of Carbocyclic Rings (9 hours)

6.1 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 Construction of macrocyclic rings-ring closing metathesis. Inter and Intramolecular Paterno-Buchi reaction: synthetic applications. 1,3 dipolar addition- synthetic applications.

6.3 Inter-conversion of ring systems (contraction and expansion)-Demjenov reaction, Migration- and Insertion-based Ring Expansions (any one approach). Electrocyclic Ring-Expansions for the construction of seven membered rings.

Textbooks

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

Reference

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

BMCH4E03: ADVANCED PHYSICAL CHEMISTRY

Credit: 3 **Total Hours: 72**

Objectives

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

- Study different computational techniques
- Understand the theory and application of diffraction and atomic absorption and emission methods
- Understand the theory, application and instrumentation of fluorescence spectroscopy method
- Appreciate the different applications of electrochemical cells
- Be aware of different electroanalytical techniques

Outcome

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

- Independently do chemistry using computers.
- Learn the theory and application of diffraction and atomic absorption and emission methods
- Learn the theory, application and instrumentation of fluorescence spectroscopy
- Study different theories and applications of electrochemistry
- Apply different electroanalytical methods

Module 1: Computational Chemistry (18 hours)

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

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

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

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

1.5 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.

1.6 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 2: Diffraction Methods and Atomic Spectroscopic Techniques (9 hours)

2.1 Electron diffraction of gases. Wierl's equation. Neutron diffraction method. Comparison of X-ray, electron and neutron diffraction methods.

2.2 Atomic absorption spectroscopy (AAS), principle of AAS, absorption of radiant energy by atoms, classification of atomic spectroscopic methods, measurement of atomic absorption, instrumentation.

2.3 Atomic emission spectroscopy (AES), advantages and disadvantages of AES, origin of spectra, principle and instrumentation.

2.4 Flame emission spectroscopy (FES), flames and flame temperature, spectra of metals in flame, instrumentation.

Reference

1. H. H. Willard, J. A. Dean, L. L. Merritt, Instrumental Methods of Analysis, 7th Edn., Imperial College Press, 2004
2. D. A. Skoog, Principles of Instrumental Analysis, Cengage, 2014.
3. D. A. Skoog, D. M. West, F. J. Holler, S. R. Crouch, Fundamentals of Analytical Chemistry, 8th Edn., Saunders College, 2007

Module 3: Fluorescence Spectroscopy (9 hours)

3.1 Characteristics of fluorescence emission, lifetime, quantum yield, quenching, resonance energy transfer, time resolved fluorescence.

3.2 Basic Instrumentation: light source, monochromator, optical filters, photomultiplier tube, polarizers.

3.3 Fluorescence sensing, mechanism of sensing, sensing techniques based on collisional quenching, energy transfer and electron transfer, examples of pH sensors. Novel fluorosphores: long lifetime metal-ligand complexes.

3.4 Basics of the following: glucose-sensing, immunoassay, protein fluorescence, Confocal fluorescence microscopy, Fluorescence correlation spectroscopy, Single-molecule fluorescence spectroscopy.

Textbooks

1. B. Valeur, Molecular Fluorescence: Principles and Applications, Wiley-VCH, 2002
2. J. R. Lakowicz, Principles of Fluorescence Spectroscopy, 3rd Edn., Springer, 2006

Module 4: Electrochemistry and Electromotive Force (18 hours)

4.1 Osmotic coefficient, ion association, fraction of association, dissociation constant, triple ion and conductance minima, equilibria in electrolytes, association constant, solubility product principle, solubility in presence of common ion, instability constant, activity coefficient and solubility measurement, determination of activity coefficient from equilibrium constant measurement.

4.2 Electrochemical cells, concentration cells and activity coefficient determination, liquid junction potential, evaluation of thermodynamic properties, the electrode double layer, electrode-electrolyte interface, different models of double layer, theory of multilayer capacity, electrocapillary, Lippmann equation, membrane potential. Lead acid cell, Lithium ion cell.

4.3 Fuel cells, classification based on working temperature, chemistry of fuel cells, H_2-O_2 fuel cells.

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

4.5 Corrosion, types, theories and methods to prevent corrosion.

Textbooks

1. 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
2. D. R. Crow, Principles and Applications of Electrochemistry, 4th Edn., Chapmann & Hall, 1994

Module 5: Electroanalytical Techniques (18 hours)

5.1 Voltametry-cyclic voltametry, ion selective electrodes, anodic stripping voltametry.

5.2 Polarography-decomposition potential, residual current, migration current, supporting electrolyte, diffusion current, polarogram, half wave potential, limiting current density, polarograph, explanation of polarographic waves.

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

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

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

5.5 Principle of glucometer, ECG and coulter counter

Textbooks

1. D. A. Skoog, D. M. West, F. J. Holler, S. R. Crouch, Fundamentals of Analytical Chemistry, 8^{th} Edn., Saunders College, 2007

Reference

1. H. H. Willard, J. A. Dean, L. L. Merritt, Instrumental Methods of Analysis, 7^{th} Edn., Imperial College Press, 2004

BMCH4E04: ADVANCED COMPUTATIONAL CHEMISTRY

Credit: 3 **Total Hours: 72**

Learning Objectives

After completing the course, students shall be able to:

- explain the most important principles for quantum chemical and molecular mechanic methods of computing the geometry and energy of molecules
- plan and apply computer-based calculations to determine the geometry, energies and electronic properties of molecules.
- describe the theory behind methods of protein sequence comparisons and protein structure comparisons
- describe theoretical methods and plan and conduct computer-based calculations of chemical properties (for example, size, hydrophobicity, dipole moment) in molecules and relate these to biological/environmental chemical effects via calculation models
- critically examine and discuss the results from computer-based computational chemistry
- present and discuss, verbally and in writing with various different groups, academic work from a societal and scientific perspective.

Module 1: Introduction to Computational Chemistry (27 hours)

1.1 Introduction: Scope of computational chemistry; course topics; review of key concepts from linear algebra. Molecular Mechanics and Force Field Methods: Basic Principles of mechanics, Concept of Force Field, Detailed study of various types of force filed and its application.

1.2 Molecular Dynamics method: Fundamental Principles, Boundary Conditions used in dynamics methods, advantages and disadvantages- applications.

1.3 Ab-Initio method: Review of quantum mechanical methods- Hartree Fock method, Concepts of basis sets – various types of basis sets and its application. Perturbation Method: Significance and applications. Semi-Empirical Method: basic principles and applications. Density Functional Theory Method: Fundamental concepts, idea of functional, brief discussion of various functional methodologies and their applications.

Reference

1. I.N. Levine, Quantum Chemistry, 6^{th} Edn., Pearson Education Inc., 2009.

2. P.W. Atkins, R.S. Friedman, Molecular Quantum Mechanics, 4th Edn., Oxford University Press, 2005.
3. D.A. McQuarrie, Quantum Chemistry, University Science Books, 2008.
4. J.H. Jensen E.G. Lewars, Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics, 2nd Edn., Springer, 2011.
5. Molecular Modeling Basics, CRC Press, 2010.

Module 2: Potential Energy Surfaces (9 hours)

2.1 Basics and significance of potential energy surfaces: The Molecular Hamiltonian, Born-Oppenheimer Approximation and its relevant mathematical details, Nuclear wave function and correlation correction. Coordinates for Potential Energy Surfaces

2.2 Characterizing Potential Energy Surfaces- stationary points, saddle points, global and local minima. Hessian Index. Introduction to geometry optimisation, single point energy, vibrational calculations and Koopmans theorem.

Reference

1. K.I. Ramachandran, G. Deepa, K. Namboori, Computational Chemistry and Molecular Modeling: Principles and Applications, Springer, 2008.
2. A. Hinchliffe, Molecular Modelling for Beginners, 2nd Edn., John Wiley & Sons, 2008.
3. C.J. Cramer, Essentials of Computational Chemistry: Theories and Models, 2nd Edn., John Wiley & Sons, 2004.
4. D.C. Young, Computational Chemistry: A Practical Guide for Applying Techniques Real-World Problems, John Wiley & Sons, 2001.

Module 3: Computer Aided Drug Designing (27 hours)

3.1 Role of Computer Aided Molecular Design in Drug Discovery. Rational Drug Design: Approaches to Rational drug designing: Analog Based studies, Pharmacophore, Structure based studies.

3.2 Molecular Properties Prediction: Drug - like Properties, Concept of Polar Surface Area, Calculation of CLOGP and its applications. ADMET properties: descriptors of absorption, distribution, metabolism, excretion and toxicity, Fragmental Methods, calculation of KLOGP, Correlation factors in CLOGP and KLOGP: structural and interaction factors.

3.3 Docking: basic principles of docking: Identification of active site: mathematical principles. Fundamentals of supramolecular interactions: hydrogen bonding, Vanderwaal's forces, dipole-dipole interaction, pi-pi stacking and ionic bonding. Calculation of interaction energy and interpretation of results.

Reference

1. Pushpendra Kumar Vishwakarma, Vikash Gupta, Leela Maharaj, Computer Aided Drug Designing, Lambert Academic Publishing, 2012.
2. Yanamala Pradeep, Analog and Structural Drug Designing on Swine Flu Inhibitors, Lambert Academic Publishing, 2011.
3. Waseem Akhtar Shamshari, Drug Designing: Homology modeling of PKC inhibitors: Computer Aided Drug designing through Homology modeling of PKC data ,known to be important class of enzyme as drug target, Lambert Academic Publishing, 2012.
4. Patric Bultinic, Computational Medicinal Chemistry for Drug Designing, Marcel Decker Publishing, 2004.

Module 4: Introduction to computational softwares (9 hours)

4.1 Quantum mechanical calculations: Introduction to Gaussian package. Concept of z-matrix for molecular specification. Model chemistry: generation of input for Gaussian calculation and interpretation of results.

4.2 Molecular Dynamics simulation: generation of molecular input: the concept of volume box, excluded volume, conversion of experimental parameters to theoretical input. Dynamics run and interpretation of results.

4.3 Docking methods: identification of target proteins/nucleic acids, calculation of active site, generation of ligand structure. Methods of docking input and its interpretation.

References

1. A. Leach, Molecular Modelling: Principles and Applications, 2nd Edn., Longman, 2001.
2. F. Jensen, Introduction to computational chemistry, 2nd Edn., John Wiley & Sons, 2007.
3. J.P. Fackler Jr., L.R. Falvello (Eds.), Techniques in Inorganic Chemistry: Chapter 4, CRC Press, 2011.

SEMESTERS III AND IV

PRACTICAL

BMCH4P04: INORGANIC CHEMISTRY PRACTICAL - II

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

PART I

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

PART II

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

Reference

1. A.I. Vogel, A Text Book of Quantitative Inorganic Analysis, Longman, 1966
2. I.M. Koltoff, E.B. Sandell, Text Book of Quantitative Inorganic Analysis, 3rd Edn., McMillian, 1968
3. G. Pass, H. Sutcliffe, Practical Inorganic Chemistry, Chapman & Hall, 1974
4. N.H. Furman, Standard Methods of Chemical Analysis: Vol. 1, Van Nostrand,1966
5. F.J. Welcher, Standard Methods of Chemical Analysis: Vol. 2, R.E. Kreiger Pub.,2006

BMCH4P05: ORGANIC CHEMISTRY PRACTICAL – II

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

1. Three Stage Synthesis (some examples)
   i. Anthranilic acid – o-chlorobenzoic acid- N-phenylanthranilic acid- acridone
   ii. o-toludine- o-chlorotoluene- o-chlorobenzoic acid- N-phenylanthranilic acid
   iii. Nitrobenzene – aniline- tribromoaniline- symm- tri bromobenzene
   iv. Benzene –nitrobenzene – hydrazobenzene- benzidine (benzidine rearrangement)
   v. Nitrobenzene – m-dinitrobenzene- m-nitroaniline- m-phenylenediamine
   vi. Benzene – nitrobenzene – azoxybenzene- azobenzene
   vii. Benzene – nitrobenzene – phenylhydroxylamine- p-aminophenol
   viii. Benzaldehyde – benzoin – benzyl- benzilic acid
   ix. Chlorobenzene - 1-chloro-2,4-dinitrobenzene – 2,4-dinitrophenol- picric acid
   x. Phthalic anhydride- o-benzoylbenzoic acid – anthraquinone- anthrone

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

(Minimum 7 preparations to be done in the lab)

2. Microwave assisted organic reactions and green chemistry synthesis (Minimum 7).
3. Synthesis of polymers.
4. TLC of organic binary mixtures with an aim to find to separate them by finding the solvent mixture for separation.
5. Quantitative separation of typical binary mixture using column chromatography.
6. Physical organic chemistry experiments.

Reference

1. A. I. Vogel, A Textbook of Practical Organic Chemistry, Longman, 1974
2. A. I. Vogel, Elementary Practical Organic Chemistry, Longman, 1958
3. G. Mann, B.C Saunders, Practical Organic Chemistry, 4^{th} Edn., 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, 3^{rd} Edn., Vikas Publications, 2013

6. V. K. Ahluwalia, Green Chemistry: Environmentally Benign Reactions, Ane Books, 2009
7. Monograph on Green Chemistry Laboratory Experiments, Green Chemistry Task Force Committee, DST, 2009

BMCH4P06: PHYSICAL CHEMISTRY PRACTICAL - II

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

(Questions from both part A and B will be asked for the examination)

Part A

I. Chemical Kinetics

1. Determination of the rate constant of the hydrolysis of ester by acid
2. Kinetics of reaction between $K_2S_2O_8$ and KI

II. Polarimetry

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

III. Refractometry

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

IV. Conductivity measurements

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

V. Potentiometry

1. Titration of a mixture of acids against a strong base
2. Determination of the concentration of a mixture of Cl^- and I^- ions

Reference

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. B. Viswanathan, Practical Physical chemistry, Viva Pub., 2005

Part B

Computational Chemistry Experiments

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

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

Reference

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. Gaussian 09 W Software, www.gaussian.com

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