ST. ALBERT’S COLLEGE (AUTONOMOUS)

ERNAKULAM

Affiliated to Mahatma Gandhi University, Kottayam, Kerala

SYLLABUS FOR POSTGRADUATE PROGRAMME

MASTER OF SCIENCE IN CHEMISTRY

UNDER CREDIT SEMESTER SYSTEM

(WITH EFFECT FROM 2022 ADMISSION)

Syllabus of M.Sc. Chemistry

Proposed by the Board of Studies on 11th March 2022

Dr. VIJAY JOHN GERSON

Chairman, Board of Studies

Approved by the Academic Council on 17th March 2022

Dr. M. A. SOLOMON, PRINCIPAL

Chairman, Academic Council

Adopted by the Governing Council on 29th March 2022

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Chairman, Governing Council

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Acknowledgement

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Dr. Vijay John Gerson

Chairman

PG Board of Studies in Chemistry

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Preface

I feel privilaged to present the syllabus for the M. Sc. Chemistry programme offered by the Department of Chemistry, St. Albert's College (Autonomous). The PG Board of Studies in Chemistry, St. Albert's College (Autonomous), has decided to revise the existing syllabus of 2019. However, it has also decided to keep the PG Regulations of 2020 unchanged. The revised syllabus of 2022 along with the regulations was accepted by the Board of Studies in its meeting held on 11th March 2022.

Dr. Vijay John Gerson
Chairman
PG Board of Studies in Chemistry

Programme Outcomes

- Critical Thinking
- Problem Solving
- Environment and Sustainability
- Self-Directed and Life Long Learning

Programme Specific Outcomes

- Acquire in-depth knowledge in chemistry through theory and practicals.
- Clear competitive exam for admission to master programmes in chemistry conducted by IITs, IISc and IISERs and other reputed institutes or universities in India and abroad.
- Be able to get job in Research and Development (R & D) as well as analytical laboratories of pharma, chemical, food products, material and plastic industries in both private and public sector.
- Be concerned and practice environmental protection and participate in sustainable development.

REGULATIONS

POST GRADUATE PROGRAMMES UNDER CREDIT SEMSTER SYSTEM, 2022

(SACA-PG-CSS 2022)

1. SHORT TITLE

1.1. These regulations shall be called SACA Regulations (2022) governing Post Graduate Programmes under Credit Semester System (SACA-PG-CSS 2022).

1.2. These Regulations shall come into force from the Academic Year 2022-2023 onwards.

2. Scope

2.1. The regulations provided herein shall apply to all regular Post-graduate programmes (except M.B.A and M.Sc. Space Science and Technology) conducted in the Institution, with effect from the academic year 2022-2023.

2.2. The provisions herein supersede all the existing regulations for the regular post-graduate programmes conducted in the Institution (except M.B.A and M.Sc. Space Science and Technology).

3. DEFINITIONS

3.1. 'Academic Council' means the Committee constituted by the Governing body under this regulation to monitor the running of the post-graduate programmes under the Credit Semester System (SACA-PG-CSS 2022).

3.2. 'Academic Week' is a unit of five working days in which distribution of work is organized from day one to day five, with five contact hours of one hour duration on each day. A sequence of minimum of 18 such academic weeks constitutes a semester.

3.3. 'Audit Course' is a course for which no credits are awarded.

3.4. 'CE' means Continuous Evaluation (Internal Evaluation)

3.5. 'Comprehensive viva-voice' means the oral examinations conducted by the appointed examiners and shall cover all courses of study undergone by a student for the programme.

3.6. 'Core Course' means a course which cannot be substituted by any other course.

3.7. 'Course' means a course segment of subject matter to be covered in a semester. Each course is to be designed variously under lectures/ tutorials/ laboratory or fieldwork/ seminar/ project/ practical training/ assignments/ viva-voice etc., to meet effective teaching and learning needs.

3.8. 'Course Code' means a unique alpha numeric code assigned to each course of a programme.

3.9. 'Course Credit' on credit of a course is defined as a minimum of 1 hour lecture /minimum of two hours lab field work per week for 18 weeks in a Semester. The course will be considered as completed only by conducting the final examination.

3.10. 'Course Teacher' means the teacher of the institution in charge of the course offered in the programme.

3.11. 'Credit (Cr)' of a course is a numerical value which depicts the measure of the weekly unit of work assigned for that course in a semester

3.12. 'Credit point (CP)' of a course is the value obtained by multiplying the Grade Point (GP) by the credit (Cr) of the course CP = GP x Cr.

3.13. 'Cumulative Grade point average (CGPA)' is the value obtained by dividing the sum of credit points of all the courses taken by the students for the entire programme by the total number of credits and shall be rounded off to two decimal places. CGPA determines the overall performance of a student at the end of the programme.
(CGPA = total CP obtained /Total credits of the programme)

3.14. 'Department' means any teaching Department in the Institution offering a programme of study approved as per the Act/ statutes of the University.

3.15. 'Department Council' means the body of all teachers of a Department in a college.

3.16. 'Dissertation' means a long document on a particular subject in connection with the project/ research/ field work etc.

3.17. 'Duration of a Programme' means the period of time required for the conduct of the programme. The duration of the post-graduate programme shall be 4 semesters spread over two academic years.

3.18. 'Elective course' means a course, which can be substituted, by an equivalent course from the same subject.

3.19. 'Elective Group' means a group consisting of elective courses for the programme.

3.20. 'ESE' means End Semester Evaluation (External Evaluation).

3.21. 'Evaluation 'is the process by which the knowledge acquired by the student is quantified as per the criteria detail in these regulations.

3.22. 'External Examiner 'is the teacher appointed from other colleges for the valuation of courses of study undergone by the students in a college. The external examiner shall be appointed by the College.

3.23. 'Exam Coordinator'is a teacher nominated by the Department Council to coordinate the continuous evaluation and other academic activities undertaken in the Department of the college.

3.24. 'Grace Grade Points' means grade points awarded to course(s), in recognition of the students' meritorious achievement in NSS/Sports/ Arts and cultural activities etc.

3.25. 'Grade point (GP) letter grade is assigned a 'Grade point' (GP) which is an integer indicating the numerical equivalent of the board level of performance of a student in a course.

3.26. 'Grade Point Average (GP)'is an index of the performance of student in a course. It is obtained by dividing the sum of the weighted grade points obtained in the course by the sum of the weights of the course. (GPA= ∑WGP/∑W).

3.27. 'Improvement course' is a course registered by a student for improving his/ her performance in that particular course.

3.28. 'Internal Examiner' is a teacher nominated by the department concerned to conduct internal evaluation.

3.29. 'Letter Grade' or 'Grade' for a course is a letter symbol (A^+, A, B^+, B, C, C^+, D) which indicates the broad level of performance of a student for a course.

3.30. 'SACA-PG-CSS 2022' means St. Albert's College (Autonomous) Regulations Governing Post Graduate Programmes under Credit Semester System, 2022.

3.31. 'Parent Department' means the Department which offers a particular post graduate programme.

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

3.33. 'Programme' means the entire course of study and examinations.

3.34. 'Project' is a core course in a programme. It means a regular project work with stated credits on which the student undergoes a project under the supervision of a teacher in the parent department/ any appropriate research center in order to submit a dissertation on the project work as specified. It allows students to work more autonomously to construct their own learning and culminate in a realistic, student-generated product for findings.

3.35. 'Repeat course' is a course that is repeated by the student for having failed in that course in an earlier registration.

3.36. 'Semester' means a team consisting of a minimum of 90 working days, inclusive of examinations, distributed over a minimum of 18 weeks of 5 working days each.

3.37. 'Seminar' means a lecture given by the student on a selected topic and is expected to train the student in self-study, collection of relevant matter from various resources, editing, document writing and presentation.

3.38. 'Semester Grade Point Average'(SGPA) is the value of trained by dividing the sum of credit points CP obtained by a student in the various courses taken in a semester by the total number of credits for the course in that semester. The SGPA shall be rounded off to two decimal places. SGPA determines the overall performance of a student at the end of the semester (SGPA= Total CP obtained in the semester /Total Credits for the semester).

3.39. '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.

3.40. 'University' means Mahatma Gandhi University, Kottayam, Kerala.

3.41. 'College' means St. Albert's College (Autonomous), Ernakulam, Kerala.

3.42. 'Weight' is a numeric measure assigned to the assessment units of various components of a course of study.

3.43. 'Weighted Grade Point' (WGP) is the grade point multiplied by weight. (WPG = GP x W).

3.44. 'Weighted Grade Point Average (WGPA)' is an index of the performance of a student in a course. It is obtained by dividing the sum of the weighted grade points by the sum of the weights. WGPA shall be obtained for CE (Continuous Evaluation) and ESE (End Semester Evaluation) separately and then the combined WGPA shall be obtained for each course.

3.45. Words and expressions used and not defined in this regulation but defined in the Mahatma Gandhi University Act and Statutes that you shall have the meaning assigned to them in the Act and Statute.

4. ACADEMIC COUNCIL: COMPOSITON OF ACADEMIC COUNCIL

4.1. The Principal (Chairman)

4.2. All Heads of the Departments

4.3. Four teachers of the college representing different categories of teaching staff by rotation on the basis of seniority of service in the college.

4.4. Not less than four experts/academicians from outside the college representing areas such as Industry, Commerce, Law, Education, Medicine, Engineering, Sciences etc., to be nominated by the Governing Body.

4.5. Three nominees of the university not less than Professors.

4.6. A faculty member nominated by the Principal (Member Secretary).

5. PROGRAMME STRUCTURE

5.1. The medium of instruction shall be English except for programmes under Faculty of Language and Literature.

5.2. Student shall be admitted to post graduate programmes under various faculties. The programme shall include two types of courses, Core courses and Elective courses. There shall be a project with the dissertation and comprehensive viva-voce as core courses for all programmes. The programme shall also include assignments/ seminars/practicals project field studyetc.

5.3. Elective course and Groups

5.3.1. There shall be at least two and not more than four elective groups (Group A, Group B, Group C, etc.) comprising of three courses each for a programme and these elective courses shall be included either in the fourth semester or be distributed among third and fourth semesters. This clause is not applicable to MSW, MBA and M. Voc.

5.3.2. The number of elective courses assigned for study in a particular semester shall be the same across all elective groups for the programme concerned.

5.3.3. The colleges shall select any one of the elective groups for each programme as per the interest of the students, availability of faculty and academic infrastructure in the Institution.

5.3.4. The selection of courses from different elective groups is not permitted.

5.3.5. The elective group selected by the college shall be intimated to the Controller of Examinations without within two weeks of commencement of the semester in which the elective courses are offered. The elective group selected by the college for the students who are admitted in a particular academic year shall not be changed.

5.4. Project work

5.4.1. Project work shall be completed in accordance with the guidelines given in the curriculum and shall be carried out under the supervision of a teacher of the department concerned. A candidate may, however, in certain cases be permitted to work on the project in an Industrial/ Research Organization on the recommendation of the supervising teacher.

5.4.2. There shall be internal assessment and external assessment for the project work.

5.4.3. The project work shall be evaluated based on the presentation of the project work done by the student, the dissertation submitted and the Viva-voce on the project.

5.4.4. The external evaluation of the project work shall be conducted by an external examiner from different college and an internal examiner from the department concerned.

5.4.5. The final Grade of the project (External) shall be calculated by taking the average of the Weighted Grade Points given by the two external examiners and the internal examiner.

5.5. **Assignments:** Every student should submit at least one assignment as an internal component for each course.

5.6. **Seminar Lecture:** Each student shall deliver one seminar lecture as an internal component for every course with a weightage of two. The seminar lecture is expected to train the student is self-study, collection of relevant matter from the various resources, editing, document writing, and presentation.

5.7. **Test Papers (Internal):** Student shall undergo at least two class tests as an internal component for each course with a weightage of one each. The best two shall be taken for awarding the grade for class tests.

5.8. No course shall have more than 5 credits unless otherwise specified.

5.9. **Comprehensive Viva-Voce**: Comprehensive Viva-voce conducted at the end of fourth semester of the programme and its evaluation shall be conducted by the examiners of the project evaluation.

5.10. Comprehensive Viva-Voce cover questions from all courses in the programme.

5.10.1. There shall be an internal assessment and an external assessment for the comprehensive Viva-voce.

6. ATTENDANCE

6.1. The minimum requirement of aggregate attendance during a semester for operating at the end-semester examination shall be 75%. Condonation of shortage of attendance for students having a minimum of 65% attendance, (upto a maximum of 10 days) in a semester subject to a maximum of two times during the whole period of the programme may be granted by the College.

6.2. If a student represents his/her institution, University, State or Nation in Sports or Cultural or any other officially sponsored activities such as College Union/ University Union etc. he/ she shall be eligible to claim the attendance for the actual number of days participated subject to a maximum of 10 days in a semester based on the specific recommendations of the teacher concerned, class tutor, Head of the Department forwarded through the Dean, Students Affairs subjected to the approval of the Principal. For exceptional achievements/situations, the Principal may recommend for the award of additional attendance to the Governing Body.

6.3. Those who could not register for the examination of a particular semester due to shortage of attendance will not be able to repeat the semester and will be removed from the rolls.

7. REGISTRATION/DURATION

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

7.2. A student who has registered for the programme shall complete the programme within a period of four years from the date of commencement of the programme.

8. ADMISSION

8.1. The admission to all regular PG programme shall be through the Centralised Allotment Process of the College.

8.2. If there is an entrance examination specified for the admission for a particular programme, it will be as per the directions of the office of the CoE of the college.

8.3. The eligibility criteria for admission to PG programmes shall be published by the College in the prospectus.

9. ADMISSION REQUIREMENTS

9.1. Candidates for admission to the first semester of the PG programme through CSS shall be required to have passed an appropriate Degree Examination of any recognized university/institutions. Other eligibility requirements for specific programmes will be published in the prospectus.

9.2. Students admitted under this programme are governed by the Regulations of the College.

10. PROMOTION

10.1. A student who registers for a particular semester examination shall be promoted to the next semester.

11. EXAMINATIONS

11.1. There shall be an examination conducted by St. Albert’s College, (Autonomous) at the end of each semester.

11.2. Practical Examination shall be conducted by the College at the end of semester or at the end of even semester as prescribed in the syllabus of the particular programme. The number of examiners for the Practical Examination shall be prescribed by the Board of Studies of the program.

11.3. End Semester Examinations: The examinations shall normally be conducted at the end of each semester.

11.4. There shall be one End-semester examination of 3 hours duration for each lecture based courses.

11.5. A question paper may contain short answer type/annotation, short essay type questions problem and long essay type questions. Different types of questions shall have different weightages.

12. EVALUATION AND GRADING

12.1. **Evaluation:** The evaluation scheme for each course shall contain two parts; (a) End Semester Evaluation (ESE) (External Evaluation) and (b) Continuous Evaluation (CE) (Internal Evaluation). The ratio of weightage between internal and external is 1:3 (unless for the courses, it is otherwise specified by the BoS). Both End Semester Evaluation (ESE) and Continuous Evaluation (CE) shall be carried out using direct grading system.

12.2. Direct grading: The direct grading for CE (Internal) and ESE (External Evaluation) shall be based on 6 letter grades (A+, A, B, C, D and E) with numerical values of 5, 4, 3, 2, 1 and 0 respectively.

12.3. Grade Point Average GPA: internal and external components are separately graded and the combined grade point with weightage 1 for internal and 3 for external shall be applied to calculate the Grade Point Average (GPA) of each course. Letter grade shall be assigned to each course based on the categorization provided.

12.4. Internal evaluation for regular programme: The internal evaluation shall be based on a predetermined transparent system involving periodic written tests, assignments, seminars, lab skills, records, Viva-voce etc.

12.5. Components of internal (CE) and external evaluation (ESE): Grades shall be given to the evaluation of theory/ practical/ project/ comprehensive Viva-voce and all internal evaluations based on the Direct Grading System.

12.6. Proper guidelines shall be prepared by the BOS for evaluating the assignment, seminar, practical, project and the comprehensive viva-voce within the framework of the regulation.

12.7. There shall be no separate minimum grade point for internal evaluation.

12.8. The model of the components and its weightages of continuous evaluation (CE) and End Semester Evaluation (ESE) are shown in below:

a) For theory (CE)(Internal)

	Components	Weightage
i.	Assignment	2
ii.	Seminar	4
iii.	Best Two Test papers	4 (2 each)
Total		**10**

(Grades of best two test papers shall be considered. For test papers all questions shall be set in such a way that the answers can be awarded A+, A, B, C, D, E grade.)

a) For the theory (ESE) (External)

Evaluation is based on the pattern of questions specified 12.16.5

b) For Practical (CE) (Internal)

Components	Weightage
Written/Lab test	2
Lab involvement and Record	1
Viva	2
Total	**5**

(The components and the weightage of the components of the practical (Internal) can be modified by the concerned BOS without changing the total weightage 5.)

a) For Practical (ESE) (External)

Components	Weightage
Written / Lab test	7
Lab involvement and Record	3
Viva	5
Total	**15**

[The components and the weightage of the practical (External) can be modified by the concerned BOS without changing the total weightage 15.]

a) For Project (CE) (Internal)

Components	Weightage
Relevance of the topic and analysis	2
Project content and presentation	2
Project viva	1
Total	**5**

(The Components and the weightage of the components of the project (Internal) can be modified by the concerned BOS without changing the total weightage 5.)

a) For Project (ESE) (External)

Components	Weightage
Relevance of the topic and analysis	3
Project content and presentation	7
Project viva	5
Total	**15**

(The Components and the weightage of the components of the project (External) can be modified by the concerned BOS without changing the total weightage 15.)

a) Comprehensive viva-voce (CE)(internal)

Components	Weightage
Comprehensive viva-voce (all courses from first semester to fourth semester)	5
Total	5

(Weightage of the components of the comprehensive viva-voce (internal) shall not be modified.)

a) Comprehensive viva-voce (CE)(External)

Components	Weightage
Comprehensive viva- voce (all courses from first semester to fourth semester)	15
Total	**15**

(Weightage of the components of the comprehensive viva-voce (external) shall not be modified unless specified by the respective BoS for a particular course.)

12.9 All grade point averages shall be rounded to two decimal points.

12.10 To ensure transparency of the evaluation process, the internal assessment grade awarded to the students in each course in a semester shall be published on the notice board at least one week before the commencement of the external examination.

12.11 There shall not be any chance for improvement for internal grade.

12.12 The course teacher and the Exam coordinator shall maintain the academic details of each student registered for the course and a copy should be kept in the department for verification for at least five years after the student completes the programme.

12.13 **External evaluation:** The external examination in theory courses is to be conducted by the College at the end of the semester. The answers should be in English expect those for the Faculty of Languages. The evaluation of the answer scripts shall be done by examiners based on a well-defined scheme of valuation. The external evaluation shall be done immediately after the examination.

12.14 Photocopies of the answer scripts of the external examination shall be made available to the students on request as per the rules prevailing in the College.

12.15 The question paper should be strictly on the basis of model question papers set and the directions prescribed by the BOS/Governing Body of the college for each programme.

12.16 **Pattern of questions**

12.16.1 Questions shall be set to access the knowledge acquired, standard application of Knowledge, application of knowledge in new situations, critical evaluation of knowledge and the ability to synthesize knowledge. Due weightages shall be given to each module based on content/ teaching hours allotted to each module.

12.16.2 The question setter shall ensure that questions covering all outcomes are met.

12.16.3 A question paper shall be a judicious mix of short answer type, short essay type/ problem solving type and long essay type questions.

12.16.4 The questions shall be prepared in such a way that the answers can be awarded A+, A, B, C, D, E grades.

12.16.5 Weight: Different types of questions shall be given different weights to quantify their range as follows:

Sl. No.	Type of Questions	Weight	Number of questions to be answered
1.	Short Answer type questions	1	8 out of 10
2	Short essay/ problem solving type questions	2	6 out of 8
3.	Long Essay type questions	5	2 out of 4

12.17 **Pattern of questions for practical**: the pattern of questions for external evaluation of practical shall be prescribed by the Board of Studies.

12.18 **Direct grading System:** Direct Grading System based on a 6-point scale is used to evaluate the Internal and External examinations taken by the students for various courses of study.

Grade	Grade Points
A+	5
A	4
B	3
C	2

D	1
E	0

12.19 Performance Grading

12.20 Students are graded based on their performance (GPA/SGPA/CGPA) at the examination on a 7-point scale as detailed below*. (7-point scale needed clarification)*

Range	Grade	Indicator
4.50 to 5.00	A+	Outstanding
4.00 to 4.49	A	Excellent
3.50 to 3.99	B+	Very good
3.00 to 3.49	B	Good(Average)
2.50 to 2.99	C+	Fair
2.00 to 2.49	C	Marginal(pass)
up to 1.99	D	Deficient (Fail)

12.21 No separate minimum is required for internal evaluation for a pass, but a minimum C grade is required for a pass in an external evaluation. However, a minimum C grade is required for pass in a course.

12.22 A student who fails to secure a minimum grade for a pass in a course will be permitted to write the examination along with the next batch.

12.23 **Improvement of course:** The candidates who wish to improve the grade/ grade point of the external examination of a course/ courses he/she has passed can do the same by appearing in the external examination of the semester concerned along with the immediate junior batch. This facility is restricted to first and second semesters of the program.

12.24 Semester Grade Point Average (SGPA) and Cumulative Grade Point Average

(CGPA) calculations. The **SGPA** is the ratio of the sum of the credit points of all courses taken by a student in the semester to the total credit for that semester. After the successful completion of a semester, Semester Grade Point Average (SGPA) of a student in that semester is calculated using the formula given below.

Semester Grade Point Average –SGPA (S_j) = $\sum(C_i \times G_i) / \sum C_i$

(SGPA = Total credit Points awarded in all semesters / Total credits of thesemester)

Where 'Sj' is the jth semester, 'Gi' is the grade point scored by the student in the ithcourse 'Ci' is the credit of ith course.

12.25 Cumulative Grade Point Average (CGPA) of a programme is calculated using the formula:-

Cumulative Grade Point Average (CGPA) =$\sum(C_i x S_i) / \sum C_i$

(CGPA = Total credit Points awarded in a semester / Total credits of the programme)

Where '**C_i**' is the credits for the **i**th semester '**S_i**' is the **SGPA** for the **i**th semester. The **SGPA** and **CGPA** shall be rounded off to 2 decimal points.

For the successful completion of semester, a student shall pass all courses and score a minimum SGPA of 2.0. However, a student is permitted to move to the next semester irrespective of her/ his **SGPA**.

13 GRADE CARD

13.1 The College under its seal shall issue to the students, a consolidated grade card on completion of the programme, which shall contain the following information.

a) Name of College

b) Name of the University

c) Title of the PG Program

d) Name of the Semesters

e) Name and Register Number of the student

f) Code, Title, Credits and Max GPA (Internal, External & Total) of each course (theory & Practical), project, viva etc., in each semester.

g) Internal, external and total grade, Grade Point (G), Letter Grade and Credit point (P) in each course opted in the semester.

h) The total credits and total credit points in each semester

i) Semester Grade Point Average (SGPA) and corresponding Grade in each semester

j) Cumulative Grade Point Average (CGPA), Grade for the entire Program.

k) Separate Grade card will be issued at the request of candidates and based on College Guidelines issued from time to time.

l) Details of description of evaluation process-Grade and Grade Point as well as indicators, calculation methodology of SGPA and CGPA as well as conversion scale shall be shown on the reverse side of the grade card.

13. AWARD OF DEGREE

The successful completion of all the courses with 'C' grade within the stipulated period shall be the minimum requirement for the award of the degree.

14. MONITORING COMMITTEE

There shall be a Monitoring Committee constructed by the Principal to monitor the internal evaluation conducted by departments.

15. POSITION CERTIFICATE

The College shall publish the list of top 3 candidates for each programme after the publication of the programme results. Position certificate shall be issued to candidates on their request.

16. Candidates shall be ranked in the order of merit based on the CGPA secured by them. Grace grade points awarded to the students shall not be counted for fixing that rank/position. Position certificates shall be signed by the Controller of Examinations.

17. GRIEVANCE REDRESSAL COMMITTEE

In order to address the grievance of students a three-level Grievance Redressal mechanism is envisaged. A student can approach the upper level only if grievance is not addressed at the lower level.

17.1. **Class Level:** The cell is chaired by the class tutor and the course teacher or a teacher nominated by the Head of the Department.

17.2. **Department level**: The College shall form a Grievance Redressal Committee in each department comprising of the course teacher and one senior teacher as members and the Head of the Department as Chairperson. The committee shall address all grievances relating to the internal assessment grade of the students.

17.3. **College level:** A committee with the Principal as Chairman, Dept. Coordinator, HOD of concerned Department and a senior teacher nominated by the Executive Committee as members.

18. TRANSITORY PROVISION

Notwithstanding anything contained in these regulations, the Governing Body shall, for a period of two 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.

19. Credits allotted for program and Courses

19.1. Total credit for each program shall be 80 Semester-wise total credit can vary from 16 to 25.

19.2. The minimum credit of a course is 2 and maximum credit is 5.

20. Course code: The course codes assigned for all courses (core courses, elective courses, common courses etc.) shall be unique.

21. Models of distribution of courses, course codes, type of the course, credits, teaching hours for a program are given in the following table.

Example Programs with the practical-Total Credits 80- scheme of the syllabus

Semester	Course Code	Course name	Type of the course	Teaching Hours Per Week	Credit	Total Credits
I	Course.code1	Name1	Core	4	4	19
	Course.code2	Name2	Core	4	4	
	Course.code3	Name3	Core	4	4	
	Course.code4	Name4	Core	3	3	
	Practical Course.code5	Name5	Core	10	4	
II	Course.code6	Name6	Core	4	4	20
	Course.code7	Name7	Core	4	4	
	Course.code8	Name8	Core	4	4	
	Course.code9	Name9	Core	3	4	
	Practical-Course.code10	Name10	Core	10	4	
III	Course.code11	Name11	Core	4	4	20
	Course.code12	Name12	Core	4	4	
	Course.code13	Name13	Core	4	4	
	Course.code14	Name14	Core	3	4	
	Practical Course.code15	Name15	Core	10	4	

IV	Course.code16	Name16	Elective	5	3	21
	Course.code17	Name17	Elective	5	3	
	Course.code18	Name18	Elective	5	3	
	Practical-Course.code19	Name19	Core	10	5	
	Project-Course.code20	Name20	Core		5	
	Comprehensive viva- voce - Course.code 21	Name 21	Core		2	
	Total					**80**

Appendix

1. Evaluation first stage-Both internal and external (to be done by the teacher)

Grade	Grade Points
A+	5
A	4
B	3
C	2
D	1
E	0

The final Grade range for courses SGPA and CGPA

Range	Grade	Indicator

4.50 to 5.00	A+	Outstanding
4.00 to 4.49	A	Excellent
3.50 to 3.99	B+	Very good
3.00 to 3.49	B	Good
2.50 to 2.99	C+	Fair
2.00 to 2.49	C	Marginal
Upto 1.99	D	Deficient(Fail)

Theory -External – ESE

Maximum weight for external evaluation is 30. Therefore, Maximum Weighted Grade Point (WGP) is 150

Type of Question	Qn. No’s	Grade Awarded	Grade point	Weights	Weighted Grade Point
Short Answer	1	A+	5	1	5
	2	-	-	-	-
	3	A	4	1	4
	4	C	2	1	2
	5	A	4	1	4
	6	A	4	1	4
	7	B	3	1	3
	8	A	4	1	4
	9	B	3	1	3
	10	-	-	-	
Short Essay	11	B	3	2	6
	12	A+	5	2	10
	13	A	4	2	8
	14	A+	5	2	10
	15	-	-	-	-
	16	-	-	-	-
	17	A	4	2	8
	18	B	3	2	6
Long Essay	20	A+	5	5	25
	21	-	-	-	-
	22	-	-	-	-
	23	B	3	5	15
			TOTAL	**30**	**117**

Calculation:

Overall Grade of the theory paper = Sum of Weighted Grade Points /Total weight 117/30 = 3.90 = Grade B

Theory- Internal-CE

Maximum weight for internal evaluation is 10. Therefore, Maximum Weighted Grade Point (WGP) is 50.

Components	Weight (W)	Grade Awarded	Grade Point(GP)	WGP= W *GP	Overall Grade of the course
Assignment	2	A	4	8	**WGP/Total weight = 48/10 =4.8**
Seminar	4	A+	5	20	
Test paper 1	2	A+	5	10	
Test paper 2	2	A+	5	10	
Total	**10**			**48**	**A+**

Practical-External-ESE

Maximum weight for external evaluation is 5. Therefore Maximum Weighted Grade Point (WPG) is 75.

Components	Weight (W)	Grade Awarded	Grade Point(GP)	WGP= W*GP	Overall Grade of the course
Written/Lab	7	A	4	28	
Test					**WGP/Total**
Lab					**weight**
Involvement &Record	3	A+	5	15	**= 58 / 15** **= 3.86**
Viva	5	B	3	15	

Total	**15**			**58**	**B**

Practical-Internal-CE

Maximum weight for internal evaluation is 5. Therefore, Maximum Weighted Grade Point (WGP) is 25

Components	Weight (W)	Grade Awarded	Grade Point(GP)	WGP=W*GP	Overall Grade of the course
Written/ Lab test	2	A	4	8	**WGP/Total weight =17/5=3.40**
Lab involvement & record	1	A+	5	5	
Viva	2	C	2	4	
Total	**5**			**17**	**B**

Project-External-ESE

Maximum weight for external evaluation is 15. Therefore, Maximum weighted Grade Point (WGP) is 75.

Components	Weight (W)	Grade Awarded	Grade Point(GP)	WGP= W*GP	Overall Grade of the course
Relevance of the topic & Analysis	2	C	2	4	**WGP/Total weight = 59/15= 3.93**
Project content & presentation	8	A+	5	40	

Project viva-voce	5	B	3	15	
Total	**15**			**59**	**B**

Project-Internal-CE

Maximum weight for Internal evaluation is 5. Therefore, Maximum Weighted Grade Point (WGP) is 25.

Components	Weight (W)	Grade Awarded	Grade Point(GP)	WGP= W *GP	Overall Grade of the course
Relevance of the topic & Analysis	2	B	3	6	**WGP/Total weight = 21/5 = 4.2**
Project content &presentation	2	A+	5	10	
Project viva-voce	1	A+	5	5	
Total	**5**			**21**	**A**

<u>Comprehensive viva-voce-External-ESE</u>

Maximum weight for External evaluation is 15. Therefore, maximum Weighted Grade Point (WGP) 75.

Components	Weight (W)	Grade Awarded	Grade Point(GP)	WGP=W*GP	Overall Grade of the course
Comprehensive viva-voce	15	A	4	60	**WGP/Total weight = 60 / 15 = 4**

Total	**15**			**60**	**A**

Comprehensive viva-Internal-CE

Maximum Weight for Internal evaluation is 5. Therefore, Maximum Weighted Grade Point (WGP) is 25.

Components	Weight (W)	Grade Awarded	Grade Point(GP)	WGP= W *GP	Overall Grade of the course
Comprehensive viva-voce	5	A+	5	25	**WGP/Total weight = 25/ 5 = 5**
Total	**5**			**25**	**A+**

Evaluation- Second stage (to be done by the College)

Consolidation of the Grade (GPA) of a Course PC-1

The End Semester Evaluation valuation (ESE) (External evaluation) grade awarded for the course PC -1 is A and its Continuous Evaluation (CE) (Internal Evaluation) grade is A. The consolidated grade for the course PC -1 is as follows:

Evaluation	Weight	Grade awarded	Grade Points awarded	Weighted Grade Point
External	3	A	4.20	12.6
Internal	1	A	4.40	4.40
Total	**4**			**17**
Grade of a course.	GPA of the course =Total weighted Grade Points/Total weight **17/4 =4.25 = Grade A**			

Evaluation- Third stage (to be done by the College)

Semester Grade Point Average (SGPA)

Course code	Title of the course	Credits (C)	Grade Awarded	Grade Points (G)	Credit Points(CP=C X G)
01	**PC-1**	**5**	**A**	**4.25**	**21.25**
02	**-----**	**5**	**A**	**4.00**	**20.00**
03	**-----**	**5**	**B+**	**3.80**	**19.00**
04	**-----**	**2**	**A**	**4.40**	**8.80**
05	**-----**	**3**	**A**	**4.00**	**12.00**
TOTAL		**20**			**81.05**
SGPA	**Total credit points / Total credits = 81.05/20 = 4.05= Grade- A**				

Evaluation-Fourth Stage (to be done by the College)

Cumulative Grade Point Average (CGPA)

If a candidate is awarded three **A+** grades in semester 1 (**SGPA** of semester 1), semester 2 (**SGPA** of semester 2) and semester 4 (**SGPA** of semester 4) and a **B** grade in semester 3 (**SGPA** of semester 3). Then the **CGPA** is calculated as follows:

Semester	Credit of the Semesters	Grade Awarded	Grade point (SGPA)	Credit points
I	20	A+	4.50	90
II	20	A+	4.60	92
III	20	B	3.00	60
IV	20	A+	4.50	90
TOTAL	**80**			**332**

CGPA= Total credit points awarded / Total credit of all semesters = 332 / 80 = 4.15 **(Which is in between 4.00 and 4.49 in 7-point scale). Therefore, the overall Grade awarded in the program is A**

Programme Design

Semester I

Sl No.	Course Code	Course Title	Course Category	Hours / Week	Total Hours	Credits
1	PCH1CRT0122	Coordination Chemistry	Core	4	72	4
2	PCH1CRT0222	Organic Chemistry - I	Core	4	72	4
3	PCH1CRT0322	Quantum Chemistry and Group Theory	Core	4	72	4
4	PCH1CRT0422	Thermodynamics , Kinetic Theory and Statistical Thermodynamics	Core	3	54	4
5	PCH1CRP0122	Inorganic Chemistry Practical-1	Core	3	54	Evaluation at the

6	PCH1CRP0222	Organic Chemistry Practical-1	Core	3	54	end of secondsemester
7	PCH1CRP0322	Physical Chemistry Practical-1	Core	4	72	
		Total		**25**	**450**	**16**

Semester II

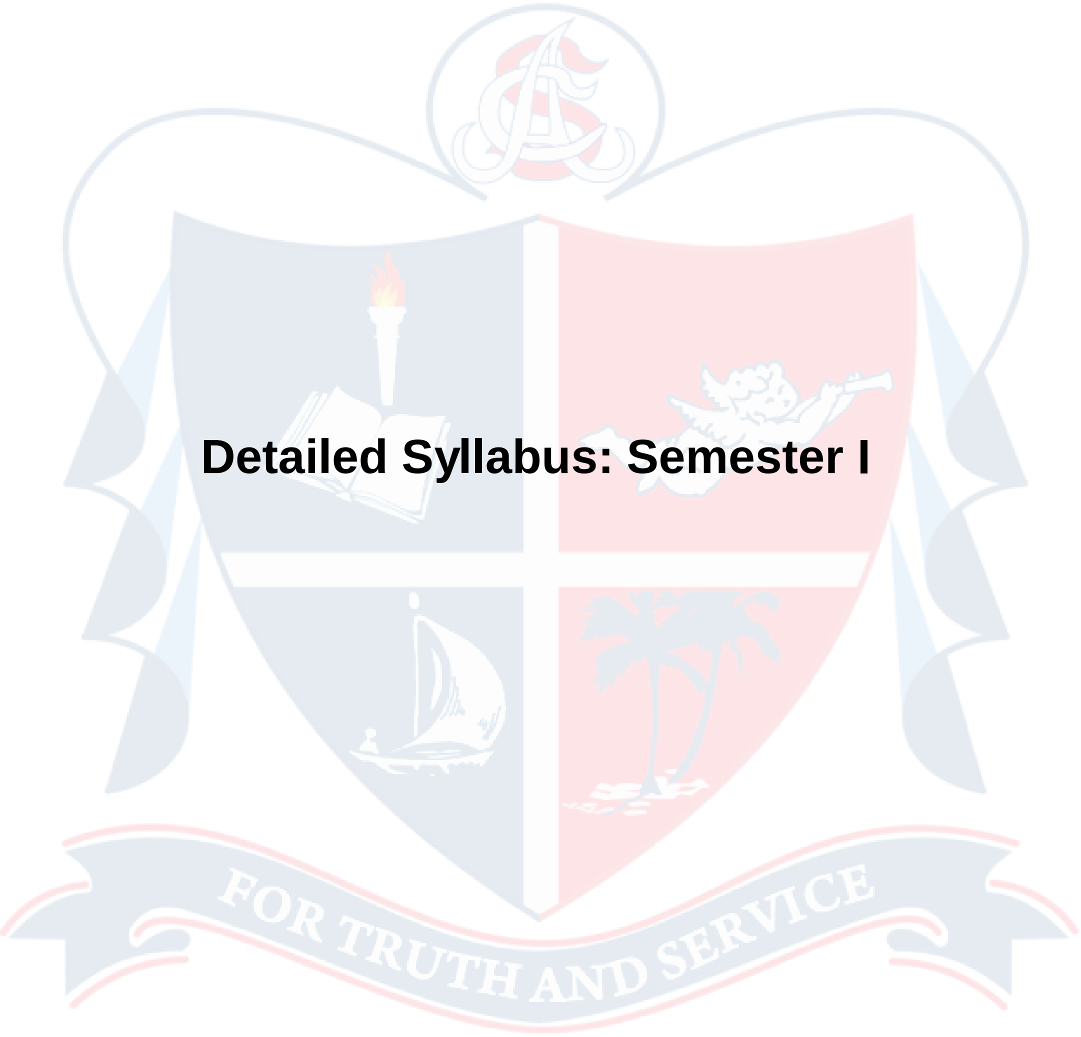
Sl No.	Course Code	Course Title	Course Category	Hours /Week	Total Hours	Credits
1	PCH2CRT0122	Organometallics and Nuclear Chemistry	Core	4	72	4
2	PCH2CRT0222	Organic Chemistry - II	Core	4	72	4
3	PCH2CRT0322	Chemical Bonding and Computational Chemistry	Core	4	72	3
4	PCH2CRT0422	Molecular Spectroscopy	Core	3	54	3
5	PCH2CRP0122	Inorganic Chemistry Practical-1	Core	3	54	3
6	PCH2CRP0222	Organic Chemistry Practical-1	Core	3	54	3
7	PCH2CRP0322	Physical Chemistry Practical-1	Core	4	72	3
		Total		**25**	**450**	**23**

Semester III

Sl No.	Course Code	Course Title	Course Category	Hours / Week	Total Hours	Credits
1	PCH3CRT0122	Structural Inorganic Chemistry	Core	4	72	4
2	PCH3CRT0222	Organic Syntheses	Core	4	72	4
3	PCH3CRT0322	Chemical Kinetics, Surface Chemistry and Crystallography	Core	4	72	4
4	PCH3CRT0422	Spectroscopic Methods in Chemistry	Core	3	54	4
5	PCH3CRP0122	Inorganic Chemistry Practical-2	Core	3	54	Evaluation at the end of fourth semester
6	PCH3CRP0222	Organic Chemistry Practical-2	Core	3	54	
7	PCH3CRP0322	Physical Chemistry Practical-2	Core	4	72	
		Total		**25**	**450**	**16**

Semester IV

Sl No.	Course Code	Course Title	Course Category	Hours / Week	Total Hours	Credits
1	PCH4CRT0122	Advanced Inorganic Chemistry	Elective	5	90	4
2	PCH4CRT0222	Advanced Organic Chemistry	Elective	5	90	4
3	PCH4CRT0322	Advanced Physical Chemistry	Elective	5	90	4
4	PCH4CPR0122	Project	Core			2
5	PCH4CRP0122	Inorganic Chemistry Practical-2	Core	3	54	3
6	PCH4CRP0222	Organic Chemistry Practical-2	Core	3	54	3
7	PCH4CRP0322	Physical Chemistry Practical-2	Core	4	72	3
8	PCH4CRV0122	Viva	Core			2
		Total		**25**	**450**	**25**



Detailed Syllabus: Semester I

COORDINATION CHEMISTRY (PCH1CRT0122)

72 Hours 4 Credits

Course Outcomes

After successful completion of the course, the students should be able to

- Explain structural aspects and bonding in coordination complexes
- Predict the spectral and magnetic properties of coordination compounds
- Explain and predict the various mechanisms associated with substitution in coordination compounds
- Outline the stereochemical aspects in coordination chemistry and apply it in chemical reactions.
- Explain the coordination chemistry of lanthanoids and actinoids

Module I: Structural Aspects and Bonding (18 Hours)

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

1.2 Splitting of d orbitals in octahedral, tetrahedral, square planar, square pyramidal and triagonal 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- M.O energy level diagrams for octahedral and tetrahedral complexes without and with π-bonding, experimental evidences for pi-bonding.

Module II: Spectral and Magnetic Properties of MetalComplexes (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^1 and d^9 ions in octahedral and tetrahedral fields (qualitative approach), d-d transitions, selection rules for electronic transitions-effect of spin orbit coupling and vibronic coupling.

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

2.3 Magnetic properties of complexes-paramagnetic and diamagnetic complexes, molar susceptibility, Gouy method for the determination of magnetic moment of complexes, spin only magnetic moment. Temperature dependence of magnetism - Curie's law, Curie-Weiss law, temperature independent paramagnetism (TIP), spin state cross over, antiferromagnetism - inter and intra molecular interaction, anomalous magnetic moments.

Module III: Kinetics and Mechanism of Reactions in Metal Complexes (18 Hours)

3.1 Thermodynamic and kinetic stability, kinetics and mechanism of nucleophilic substitution reactions in square planar complexes - trans effect-theory and applications, effect of entering ligand, effect of leaving group and effect of ligands already present on reaction rate, effect of solvent and reaction pathways, substitution in tetrahedral and five-coordinate complexes.

3.2 Kinetics and mechanism of octahedral substitution- water exchange, dissociative and associative mechanisms, interchange mechanisms and various mechanistically activation processes, base hydrolysis, racemization reactions, solvolytic reactions (acidic and basic).

3.3 Electron transfer reactions: Outer sphere mechanism-Marcus theory, inner sphere mechanism -Taube mechanism, mixed outer and inner sphere reactions, two electron transfer and intramolecular electron transfer.

Module IV: Stereochemistry of Coordination Compounds (9 Hours)

4.1 Geometrical and optical isomerism in octahedral complexes, resolution of optically active complexes, determination of absolute configuration of complexes by ORD and circular dichroism, stereoselectivity and conformation of chelate rings, asymmetric synthesis catalyzed by coordination compounds,

4.2 Linkage isomerism: Electronic and steric factors affecting linkage isomerism, symbiosis-hard and soft ligands, Prussian blue and related structures, Macrocycles- crown ethers.

Module V: Coordination Chemistry of Lanthanoids and Actinoids (9 Hours)

5.1 Term symbols for lanthanide ions, inorganic compounds and coordination complexes of the lanthanoids upto coordination No.12, electronic spectra and magnetic properties of lanthanoid complexes, organometallic complexes of the lanthanoids- σ-bonded complexes, cyclopentadienyl complexes, organolanthanoid complexes as catalysts.

5.2 General characteristics of actinoids-difference between 4f and 5f orbitals, coordination complexes of the actinoids - sandwich complexes, coordination complexes and organometallic compounds of thorium and uranium, comparative account of coordination chemistry of lanthanoids and actinoids with special reference to electronic spectra and magnetic properties.

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ORGANIC CHEMISTRY – I (PCH1CRT0222)

72 Hours 4 Credits

Course Outcomes

After successful completion of the course, the students should be able to

- Explain various basic and advanced concepts of aromaticity and apply it to substitution reactions
- Explain and apply various aspects of physical organic chemistry like Hammet equation, HSAB concepts etc.
- Acquire problem solving skills with regard to fundamental organic photochemical reactions.
- Acquire advanced level of recognition of stereochemistry including their predictions in reactions
- Recognize various conformations and their consequences in organic chemistry

Module I: Basic Concepts in Organic Chemistry (18 Hours)

1.1 Review of basic concepts in organic chemistry: Bonding, hybridisation, MO picture of butadiene and allyl systems.

1.2 Electron displacement effects: Inductive effect, electromeric effect, resonance effect, hyperconjugation, steric effect. Bonding weaker than covalent bonds.

1.3 Concept of aromaticity: Delocalization of electrons - Hückel's rule, criteria for aromaticity, examples of neutral and charged aromatic systems - annulenes. NMR as a tool ,carbon nanotubes and graphene

1.4 Mechanism of electrophilic and nucleophilic aromatic substitution reactions with examples. Arenium ion intermediates. SN1, SNAr, SRN1 and benzyne mechanisms.

Module II: Physical Organic Chemistry (9 Hours)

2.1 Energy profiles. Kinetic versus thermodynamic control of product formation, Hammond postulate, kinetic isotope effects with examples. Linear free energy relationships-Hammet equation, Taft equation.

2.2 Catalysis by acids, bases and nucleophiles with examples from acetal, cyanohydrin. Ester formation and hydrolysis reactions of esters - AAC2, AAC1, AAL1, BAC2 and BAL1 mechanisms. Hard and soft acids, bases - HSAB principle and its applications (organic reactions only)

Module III: Organic Photochemistry (9 Hours)

3.1 Photoreactions of carbonyl compounds: Norrish reactions of ketones. Patterno-Buchi reaction. Barton (nitrite ester reaction); Di-π-methane and Photo Fries rearrangements, photochemistry of conjugated dienes (butadiene only), photochemistry of vision.

Module IV: Stereochemistry of Organic Compounds (18 Hours)

4.1 Stereoisomerism: Definition based on symmetry and energy criteria, configuration and conformational stereoisomers, introduction to Atropisomerism

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

4.3 Axial, planar and helical chirality with examples, stereochemistry and absolute configuration of allenes, biphenyls and binaphthyls, ansa and cyclophanic compounds, spiranes, exo-cyclic alkylidene cycloalkanes.

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

4.5 Geometrical isomerism: nomenclature, E-Z notation, methods of determination of geometrical isomers, interconversion of geometrical isomers.

Module V: Conformational Analysis (18 Hours)

5.1 Conformational descriptors: Factors affecting conformational stability of molecules, conformational analysis of substituted ethanes, cyclohexane and its derivatives, decalins, adamantine and norbornane.

5.2 Conformation and reactivity of elimination (dehalogenation, dehydrohalogenation, semipinacolic deamination and pyrolytic elimination - Saytzeff and Hofmann eliminations), substitution and oxidation of 2^{o} alcohols.

5.3 Chemical consequence of conformational equilibrium - Curtin Hammett principle.

References

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2. F.A. Carey, R.A. Sundberg, Advanced Organic Chemistry, Part A: Structure and Mechanisms, 5th Edn., Springer, 2007.
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QUANTUM CHEMISTRY AND GROUP THEORY (PCH1CRT0322)

72 Hours 4 Credits

Course Outcomes

After successful completion of the course, the students should be able to

- Recognize the importance of symmetry and symmetry elements
- Recognize the importance of point groups and able to categorise common molecules into various point groups
- Acquire basic concepts of quantum mechanics
- Explain the postulates of quantum mechanics and recognize their importance
- Uplift knowledge in quantum mechanics to various application levels

Module I: Group Theory and Applications in Chemical Bonding (36 Hours)

1.1 Symmetry elements and symmetry operations.

1.2 Determination of point groups of molecules and ions (organic / inorganic / complex) belonging to C_n, C_s, C_i, C_{nv}, C_{nh}, $C_{\infty v}$, D_{nh}, $D_{\infty h}$, D_{nd}, T_d and O_h pointgroups.

1.3 Symmetry in crystals: 32 crystallographic point groups (no derivation), Hermann-Mauguin symbols. Screw axis-pitch and fold of screw axis, glide planes,space groups (elementary idea only)

1.4 Mathematical groups: Properties, Abelian groups, cyclic groups, sub groups, similarity transformation, classes - C_{2v}, C_{3v} andC_{2h}.

1.5 Group multiplication tables (GMTs) - C_{2v}, C_{3v} and C_{2h}, isomorphic groups.

1.6 Matrix representation of elements like E,Cn, Sn, I, σ-matrix representation of point groups like C_{2v},C_{3v},C_{2h},C_{4v} - trace /character, block factored matrices.

1.7 Reducible and irreducible representations, standard reduction formula, statement of great orthogonality theorem (GOT), construction of character tables for C_{2v}, C_{2h}, C_{3v} andC_{4v}.

1.8 Application in chemical bonding: Projection operator, transformation properties of atomic orbitals, construction of symmetry adapted linear combination of atomic orbitals (SALCs) of C_{2v}, C_{3v},D_{3h} and C_{2h} molecules.

Module II Quantum Mechanics and Applications (36 Hours)

2.1 Experimental foundation of quantum mechanics: Elementary ideas of black body radiation, photoelectric effect and atomic spectra. Need of quantum mechanics. Concept of matter wave, de Broglie relation, uncertainty principle and its consequences.

2.3 Postulates of Quantum Mechanics: State function or wave function postulate: Born interpretation of the wave function, well behaved functions, orthonormality of wave functions. Operator postulate: Operator algebra, linear and nonlinear operators, Laplacian operator, commuting and noncommuting operators, Hermitian operatorsand their properties, Eigen functions and Eigen values of an operator. Eigen value postulate: Eigen value equation, Eigen functions of commuting operators. Expectation value postulate. Postulate of time-dependent Schrödinger equation, conservative systems and time-independent Schrödinger equation.

2.4 Translational motion: Free particle in one-dimension, particle in a one dimensional box with infinite potential walls, particle in a one-dimensional box with finite potential walls-tunneling, particle in a three dimensional box, separation of variables, degeneracy.

2.5 Vibrational motion: One-dimensional harmonic oscillator (complete treatment), Hermite equation (solving by method of power series), Hermite polynomials, recursion relation, wave functions and energies-important features, harmonic oscillator model and molecular vibrations.

2.6 Rotational motion: Co-ordinate systems, Cartesian, cylindrical polar and spherical polar coordinates and their relationships. The wave equation in spherical polar coordinates-particle on a ring, the phi equation and its solution, wave functions in the real form. Non-planar rigid rotor (or particle on a sphere), separation of variables, the phi and the theta equations and their solutions, Legendre and associated Legendre equations, Legendre and associated Legendre polynomials. Spherical harmonics (imaginary and real forms), polar diagrams of spherical harmonics.

2.7 Quantization of angular momentum, quantum mechanical operators corresponding to angular momenta (Lx, Ly, Lz and L^2), commutation relations between these operators. Spherical harmonics as Eigen functions of angular momentum operators Lz and L^2. Ladder operator method for angular momentum, space quantization.

2.8 Quantum Mechanics of Hydrogen-like Atoms: Potential energy of hydrogen-like systems. The wave equation in spherical polar coordinates: separation of variables-r, theta and phi equations and their solutions, wave functions and energies of hydrogen- like atoms. Orbitals: Radial functions, radial distribution functions, angular functions and their plots. Dirac's relativistic equation for hydrogen atom (Elementary ideaonly).

2.9 Spin orbitals: Construction of spin orbitals from orbitals and spin functions, spin orbitals for many electron atoms, symmetric and antisymmetric wave functions. Pauli's exclusion principle, slater determinants.

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THERMODYNAMICS, KINETIC THEORY AND STATISTICALTHERMODYNAMICS (PCH1CRT0422)

54 Hours 4 Credits

Course Outcomes

After successful completion of the course, the students should be able to

- Able to apply principles and laws of equilibrium thermodynamics to multicomponent systems
- Calculate thermodynamic properties of ideal gases and real gases
- Analyze the advanced aspects with regard to kinetic theory of gases and find solutions to problems related to it.

ModuleI: Classical Thermodynamics (18 Hours)

1.1 Mathematical foundations for thermodynamics-variables of thermodynamics, extensive and intensive quantities, equation for total differential, conversion formulas, exact differentials-general formulation, reciprocity characteristics, homogeneous functions, Euler'stheorem.(Non-evaluative)

1.2 Thermodynamic equations of state. Maxwell relations and significance, irreversible processes - Clausius inequality.

1.3 Free energy, thermodynamic equilibria and free energy functions, temperature dependence of free energy - Gibbs Helmholtz equation, applications of Gibbs Helmholtz equation.

1.4 Partial molar quantities, chemical potential and Gibbs-Duhem equations, variation of chemical potential with temperature and pressure, determination of partial molar volume and enthalpy.

1.5 Fugacity, relation between fugacity and pressure, determination of fugacity of a real gas, variation of fugacity with temperature and pressure. Activity, dependence of activity on temperature and pressure.

1.6 Thermodynamics of mixing, Gibbs-Duhem-Margules equation, applications of

Gibbs- Duhem- Margules equation- Konovalov's first and second laws, excess thermodynamic functions - free energy, enthalpy, entropy and volume, determination of excess enthalpy andvolume.

1.7 Chemical affinity and thermodynamic functions, effect of temperature and pressure on chemical equilibrium- Vant Hoff reaction isochore andisotherm.

1.8 Third law of thermodynamics, Nernst heat theorem, determination of absolute entropies using third law.

1.9 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.

Module II: Kinetic Theory of Gases (9 Hours)

2.1 Derivation of Maxwell's law of distribution of velocities, graphical representation, experimental verification of the law, most probable velocity, derivation of average, RMS and most probable velocities, collision diameter, collision frequency, mean free path, effusion, the rate of effusion, time dependence of pressure of an effusing gas, the law of corresponding states, transport properties of gases.

Module III:Statistical Thermodynamics (27 Hours)

3.1 Brief history about the macroscopic and microscopic approach in science, permutation, probability, Stirling's approximation, macrostates and microstates, equal-apriori principle and thermodynamic probability, phase-space, ensemble, types of ensembles.

3.2 Boltzmann distribution law, partition function and its physical significance, relation between molecular partition function and molar partition function, distinguishable and indistinguishable particles, partition function and thermodynamic functions, separation of partition function-translational, rotational, vibrational, and electronic partition functions, partition function for hydrogen.Thermal de-Broglie wavelength

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

3.4 Need for quantum statistics, Bosons and Fermions, Bose-Einstein statistics:, Bose- Einstein distribution law, Bose-Einstein condensation, first order and higher order phase transitions, liquid helium, Fermi- Dirac statistics, Fermi- Dirac distribution law, application in electron gas, thermionic emission. Comparison of three statistics.

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

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1. Irving M. Klotz, Robert M.Rosenberg, Chemical Thermodynamics,John Wiley & Sons,INC Publication,2008
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6. G.W. Castellan, Physical Chemistry, Addison-Wesley, 1983.
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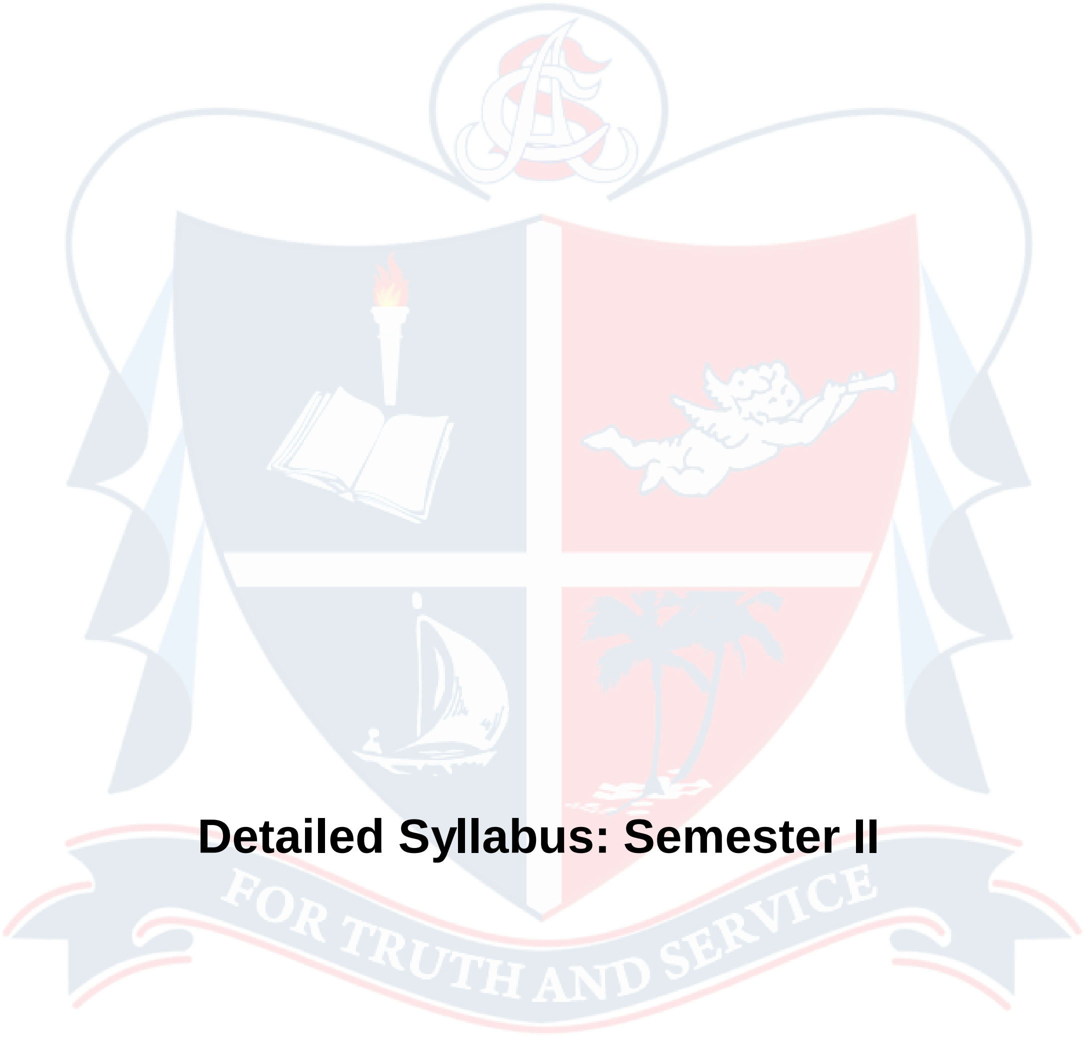

Detailed Syllabus: Semester II

ORGANOMETALLICS AND NUCLEAR CHEMISTRY (PCH2CRT0122)

72 Hours 4 Credits

Course Outcomes

After successful completion of the course, the students should be able to

- Explain the basic concepts in organometallic chemistry
- Recognze the various reactions associated with organometallic compounds
- Recognize the industrial processes catalyzed by organometallic complexes
- Recognize and explain the role of inorganic chemistry in biological systems
- Explain various aspects of radioactivity

Module I: Organometallic Compounds-Synthesis, Structure and Bonding

(18 Hours)

1.1 Haptonomenclature of organometallic compounds, organometallic compounds with linear pi donor ligands-olefins, acetylenes, dienes and allyl complexes-synthesis, structure andbonding.

1.2 Synthesis and structure of complexes with cyclic pi donors, metallocenes and cyclic arene complexes, bonding in ferrocene and dibenzenechromium, carbene including NHCand carbyne complexes.

1.3 Metal carbonyls: CO as a pi-bonding ligand, synergism, preparation, properties, structure and bonding of simple mono and binuclear metal carbonyls, metal nitrosyls, metal cyanides and dinitrogen complexes. Polynuclear metal carbonyls with and without bridging. Carbonyl clusters-LNCCS and HNCCS, Isoelectronic and isolobal analogy, Wade-Mingos rules, cluster valence electrons. IR spectral studies of bridging and non-bridging CO ligands.

1.4 Metal phosphines, hydrides and dihydrogen complexes.

Module II: 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- concerted addition, S_N2, radical and ionic mechanisms. Reductive elimination- binuclear reductive elimination and σ-bond metathesis.Oxidative coupling and reductive decoupling. Insertion (migration) and elimination reactions – insertions of CO and alkenes, insertion into M−H versus M−R, α, β, γ and δ eliminations.

2.3 Redistribution reactions, fluxional isomerism of allyl, cyclopentadienyl and allene systems.

Module III: Catalysis by Organometallic Compounds (18 Hours)

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

3.2 Reactions of carbon monoxide and hydrogen-the water gas shift reaction, the Fischer- Tropsch reaction (synthesis of gasoline).

3.3 Hydroformylation of olefins using cobalt and rhodium catalysts.

3.4 Polymerization by organometallic initiators and templates for chain propagation-Ziegler Natta catalysts, polymerisation by metallocenecatalysts.

3.5 Carbonylation reactions: Monsanto acetic acid process, olefin hydroformylation-oxo process, carbonylation of alkenes and alkynes in the presence of a nucleophile- the Reppe reaction.

3.6 Olefin methathesis-ROMP

3.7 Oxidation of olefins: Palladium catalysed oxidation of ethylene- the Wacker process,epoxidation of olefins, hydroxylation by metal-oxocomplexes

3.8 Asymmetric catalysis- Asymmetric hydrogenation-Enantioselective hydrogenatios in the synthesis of L-DOPA, Naproxen, levofloxacin, (S)-Metalachlor, isomerisation andepoxidation.

3.9 C-H activation and functionalization of alkanes and arenes: Radical type oxidation, hydroxylation, dehydrogenation, carbonylation and regioselective borylation of alkanes and cycloalkanes. Radical type reactions, electrophilic reactions, carbonylation and borylation of arenes. Insertion of alkenes and alkynes in the Ar-H bond.

3.10 Oxidative coupling reactions of alkynes with other unsaturated fragments for the formation of cyclic and heterocylic compounds. The Dӧtzreaction.

Module IV:Bio-inorganic Compounds (18 Hours)

4.1 Essential and trace elements in biological systems, toxic effects of metals (Cd, Hg, Cr,Pb and As), structure and functions of biological membranes, mechanism of ion transport across membranes, sodium-potassium pump, ionophores, valinomycin. Phosphate esters in biology, Redox metalloenzymes, cytochromes-cytochrome P-450.

4.2 Oxygen carriers and oxygen transport proteins: Structure and functions of haemoglobins and myoglobin, oxygen transport mechanism, cooperativity, Bohr effect. Structure and functions of haemerythrins and haemocyanin.

4.3 Biochemistry of zinc and copper: Structure and functions of carbonic anhydrase, carboxypeptidase A and superoxide dismutase.

4.4 Other important metal containing biomolecules: Vitamin B_{12} and the vitamin B_{12} coenzymes, photosynthesis-chlorophyll a, PS I and PSII.

4.5 Role of calcium in muscle contraction, blood clotting mechanism and biological calcification. Metals in medicine-therapeutic applications of cis-platin, radioisotopes and MRI agents.

Module V: Nuclear Chemistry (9 Hours)

5.1 Nuclear Reactions: Q value and reaction threshold, reaction cross section, cross section and reaction rate, neutron capture cross section- variation of neutron capture cross section with energy (1/V law). Nuclear fission - fission fragments and mass distribution, fission yields, fission energy, fission cross section and threshold fission neutrons, nuclear fusion reactions and their applications.

5.2 Principles of counting technique: G.M. counter, proportional, ionization and scintillation counters, cloud chamber.

5.3 Synthesis of transuranic elements: Neptunium, Plutonium, Curium, Berkelium, Einsteinium, Mendelevium, Nobelium,Lawrencium

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

5.5 Radiation chemistry of water and aqueous solutions. Measurement of radiation doses. Relevance of radiation chemistry in biology, organic compounds and radiation polymerization.

References

1. J.E. Huheey, E.A. Keiter, R.L. Keiter, Inorganic Chemistry Principles of Structure and Reactivity, 4th Edn., Harper Collins College Publishers,1993.
2. F.A. Cotton, G. Wilkinson, C.A. Murillo, M. Bochmann, Advanced Inorganic Chemistry, 6th edition, Wiley-Interscience,1999.
3. K.F. Purcell, J.C. Kotz, Inorganic Chemistry, Holt-Saunders, 1977.
4. P. Powell, Principles of Organometallic Chemistry, 2nd Edn., Chapman and Hall,1988.
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6. B.D. Guptha, A.J Elias, Basic Organometallic Chemistry, Universities Press, 2010.
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8. Sumit Bhaduri, Doble Mukesh, Homogeneous Catalysis: Mechanism and

Industrial Applications, Wiley Interscience, 2000.

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10. Robert H. Crabtree, The Organometallic Chemistry of the Transition Metals, 4thEdn., Wiley Interscience, 2005.
11. R. M. Roat-Malone, Bioinorganic Chemistry A Short Course, Wiley Interscience, 2007.
12. Robert R. Crichton, Biological Inorganic Chemistry A New Introduction to Molecular Structure and Function, Elsevier, 2012.
13. H.J. Arnikar, Essentials of Nuclear Chemistry, Wiley Eastern, 1982.
14. S.N. Goshal, Nuclear Physics, S. Chand and Company, 2006.

ORGANIC CHEMISTRY - II (PCH2CRT0222)

72 Hours 4 Credits

Course outcomes

After successful completion of the course, the students should be able to

- Re call and recognize various organic reaction mechanisms
- Explain and apply the chemistry of carbanions, carbocations, carbenes, carbenoids, nitrenes and arynes
- Illustrate and apply the chemistry of radical intermediates
- Summarize and apply the chemistry of carbonyl compounds
- Recognize concerted reactions and apply it suitably to solve problems

Module I: Review of Organic Reaction Mechanisms (9 Hours)

1.1 Review of organic reaction mechanisms with special reference to nucleophilic and electrophilic substitution at aliphatic carbon (SN_1, SN_2, SN_i, SE_1, SE_2), elimination (E_1 and E_2) and addition reactions (regioselectivity: Markovnikov's addition-carbocation mechanism, anti-Markovnikov's addition-radical mechanism). Elimination vs substitution.

1.2 A comprehensive study on the effect of substrate, reagent, leaving group, solvent and neighbouring group on nucleophilic substitution (SN_2 and SN_1) and elimination (E_1 and E_2) reactions.

Module II: Chemistry of Carbanions (9 Hours)

2.1 Formation, structure and stability of carbanions; Reactions of carbanions: C-X bond (X = C, O, N) formations through the intermediary of carbanions. Chemistry of enolates and enamines.Kinetic and Thermodynamic enolates - lithium and boron enolates in aldol and Michael reactions, alkylation and acylation of enolates.

2.2 Nucleophilic additions to carbonyls groups: Named reactions under carbanion chemistry-mechanism of Claisen, Dieckmann, Knoevenagel, Stobbe, Darzen and acyloin condensations, Shapiro reaction and Julia elimination. Favorski rearrangement.

2.3 Ylids: chemistry of phosphorous and sulphurylids - Wittig and related reactions, Peterson olefination.

Module III: Chemistry of Carbocations (9 Hours)

3.1 Formation, structure and stability of carbocations. Classical and non-classical carbocations.

3.2 C-X bond (X = C, O, N) formations through the intermediary of carbocations. Molecular rearrangements including Wagner-Meerwein, Pinacol-pinacolone, Semi- pinacol, Dienone-phenol and Benzilic acid rearrangements, Noyori annulation, Prins reaction.

3.3 C-C bond formation involving carbocations: Oxymercuration, Halolactonisation.

Module IV: Carbenes, Carbenoids, Nitrenes and Arynes (9 Hours)

4.1 Structure of carbenes (singlet and triplet), generation of carbenes, addition and insertionreactions.

4.2 Reactions of carbenes such as Wolff rearrangement, Reimer-Tiemann reaction. Reactions of ylides by carbenoid decomposition

4.3 Structure, generation and reactions of nitrene and related electron deficient nitrene intermediates.

4.4 Hoffmann, Curtius, Lossen, Schmidt and Beckmann rearrangement reactions.

4.5 Arynes: Generation, structure, stability and reactions. Orientation effect - amination of haloarenes.

Module V: Radical Reactions (9 Hours)

5.1 Generation of radical intermediates and its (a) addition to alkenes, alkynes (inter and intramolecular) for C-C bond formation - Baldwin's rules (b) fragmentation and rearrangements - Hydroperoxide: formation, rearrangement and reactions. Auto oxidation.

5.2 Name reactions involving radical intermediates: Barton deoxygenation and decarboxylation, McMurry coupling.

Module VI: Chemistry of Carbonyl Compounds (9 Hours)

2.1 Reactions of carbonyl compounds: Oxidation, reduction (Clemmensen and Wolf-Kishner), addition (addition of cyanide, ammonia, alcohol) reactions, Aldol condensation, Cannizzaro reaction, Addition of Grignard reagent. Structure and reactions of α, β- unsaturated carbonyl compounds involving electrophilic and nucleophilic addition - Michael addition, Mannich reaction, Robinson annulation.

Module VII: Concerted Reactions (18 Hours)

7.1 Electrocyclic, sigmatropic, cycloaddition, chelotropic, ene and dyotropic reactions. Woodward Hoffmann rules - Frontier orbital and orbital symmetry correlation approaches - PMO method (for electrocyclic and cycloaddition reactionsonly).

7.2 Highlighting pericyclic reactions in organic synthesis such as Claisen, Cope, Wittig, Mislow-Evans and Sommelet-Hauser rearrangements. Diels-Alder and Ene reactions (with stereochemical aspects), dipolar cycloaddition.

7.3 Unimolecular pyrolytic elimnination reactions: Cheletropic elimination, decomposition of cyclic azo compounds, β-eliminations involving cyclic transition states such as N-oxides (Cope reaction), Acetates and Xanthates (Chugaeve reaction).

7.4 Problems based on the above topics

References

1. R. Bruckner, Advanced Organic Chemistry: Reaction Mechanism, Academic Press, 2002.
2. F.A. Carey, R.A. Sundberg, Advanced Organic Chemistry, Part B: Reactions and

Synthesis, 5th Edn., Springer, 2007.

3. W. Carruthers, I. Coldham, Modern Methods of Organic Synthesis, Cambridge University Press, 2005.
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5. Fleming, Frontier Orbitals and Organic Chemical Reactions, Wiley,1976.
6. S. Sankararaman, Pericyclic Reactions-A Text Book, Wiley VCH, 2005.
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8. J. Clayden, N. Greeves, S. Warren, P. Wothers, Organic Chemistry, Oxford University Press, 2004.

CHEMICAL BONDING AND COMPUTATIONAL CHEMISTRY (PCH2CRT0322)

72 Hours 3 Credits

Course Outcomes

After successful completion of the course, the students should be able to

- Apply suitably group theory in spectroscopy
- Learn various approximation methods in quantum mechanics
- Elucidate chemical bondings in the perspective of quantum mechanics
- Learn basic concepts in computational chemistry
- Recognize various methods of computational calculations

Module I: Application of Group Theory in Spectroscopy (18 Hours)

1.1 Vibrational mode analysis using group theory taking H_2O, NH_3 and trans-N_2F_2 as examples using symmetry coordinates and internal coordinates method, prediction of IR and Raman activity,-rule of mutual exclusion,-redundant modes, out of plane modes.

1.2 Application in uv-visible spectroscopy, selection rules, orbital selection rules, transitions between non-degenerate states, prediction of electronic transitions in C_{2v},C_{3v},C_{4v},C_{2h} and C_{4h} using direct product terms , spin selection rules, relaxation in selection rules and distortion.

1.3 Application in hybridization,determination of hybridization and hybrid functions in CH_4, BF_3 and PCl_5

1.4 Group theory and optical activity (brief study)

Module II: Approximation Methods in Quantum Mechanics (18 Hours)

2.1 Many-body problem and the need of approximation methods, independent particle model. Variation method:Variation theorem with proof, illustration of variation theorem using the trial function x(a-x) for particle in a 1D-box and using the trial function $e^{-\alpha r}$ for the hydrogen atom, variation treatment for the ground state of helium atom.

2.2 Perturbation method, time-independent perturbation method (non-degenerate case only), first order correction to energy and wave function, illustration by application to particle in a 1D-box with slanted bottom, perturbation treatment of the ground state of the helium atom. Qualitative idea of Hellmann-Feynman theorem.

2.3 Hartree-Fock method, multi-electron atoms. Hartree-Fock equations (no derivation). The Fock operator, core hamiltonian, coulomb operator and exchange operator.Qualitative treatment of Hartree-Fock Self-Consistent Field (HFSCF) method. Roothan's concept of basis functions, Slater type orbitals (STO) and Gaussian type orbitals (GTO), sketches of STO and GTO.

Module III: Chemical Bonding (18 Hours)

3.1 Schrödinger equation for molecules. Born-Oppenheimer approximation, valence bond (VB) theory, VB theory of H_2 molecule, singlet and triplet state functions (spin orbitals) of H_2.

3.2 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, comparison of MO and VB theories.

3.3 Hybridization, quantum mechanical treatment of sp, sp^2 and sp^3 hybridisation. Semiempirical MO treatment of planar conjugated molecules, Hückel Molecular Orbital (HMO) theory of ethene, allyl systems, butadiene and benzene. Calculation of charge distributions, bond orders and freevalency.

Module IV: Computational Chemistry (18 Hours)

4.1 Introduction and scope of computational chemistry, potential energy surface, conformational search, global minimum, local minima, saddle points.

4.2 Ab initio methods: A review of Hartee-Fock method, self-consistent field (SCF) procedure. Roothan concept basis functions.Basis sets and its classification: Slater type and Gaussian type basis sets, minimal basis set, Pople style basis sets. Hartree-Fock limit. Post Hartree-Fock methods - introduction to Møller Plesset perturbation theory, configuration interaction, coupled cluster and semi empirical methods.

4.3 Introduction to Density Functional Theory (DFT) methods: Hohenberg-Kohn theorems, Kohn-Sham orbitals, exchange correlation functional, local density approximation, generalized gradient approximation, hybrid functionals (only the basic principles and terms need to be introduced).

4.4 Comparison of ab initio, semi empirical and DFTmethods.

4.5 Molecular geometry input: Cartesian coordinates and internal coordinates, Z matrix, Z-matrix of single atom, diatomic molecule, non-linear triatomic molecule, linear triatomic molecule, polyatomic molecules like ammonia, methane and ethane. General format of GAMESS / Firefly input file, single point energy calculation, geometry optimization, constrained optimization and frequency calculation. Koopmans' theorem.

4.6 Features of molecular mechanics force field-bond stretching, angle bending, torsional terms, non-bonded interactions and electrostatic interactions. Commonly used force fields- AMBER andCHARMM.

References

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2. P.W. Atkins, R.S. Friedman, Molecular Quantum Mechanics, 4th Edn., Oxford University Press,2005.
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4. J.P. Lowe, K Peterson, Quantum Chemistry, 3rd Edn., Academic Press, 2006.
5. R. Anatharaman, Fundamentals of Quantum Chemistry, Macmillan India, 2001.
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20. C.J. Cramer, Essentials of Computational Chemistry: Theories and Models, 2nd Edn., John Wiley & Sons,2004.
21. D.C. Young, Computational Chemistry: A Practical Guide for Applying Techniques to RealWorld Problems, John Wiley & Sons, 2001.
22. Softwares
23. MolecularMechanics:

24. Arguslab, Tinker, NAMD, DL-POLY, CHARMM, AMBER
25. Ab initio, semiempirical anddft:Firefly / PC GAMESS available fromhttp://classic.chem.msu.su/gran/gamess/
26. WINGAMESS available fromhttp://www.msg.ameslab.gov/gamess/
27. Graphical User Interface(GUI):Gabedit available fromhttp://gabedit.sourceforge.net/ 2.wxMacMolPlt available fromhttp://www.scl.ameslab.gov/MacMolPlt

MOLECULAR SPECTROSCOPY (PCH2CRT0422)

54 Hours 3 Credits

Course Outcomes

After successful completion of the course, the students should be able to

- Recognize and explain the foundations of spectroscopic techniques
- Explain the theoretical aspects of microwave spectroscopy
- Explain the theoretical aspects of infra red spectroscopy
- Explain the theoretical aspects of electronic spectroscopy
- Explain the theoretical aspects of NMR and ESR spectroscopy

Module I: Foundations of Spectroscopic Techniques (3 Hours)

1.1 Regions of the electromagnetic radiation, origin of spectrum, intensity of absorption, signal to noise ratio, natural line width. Doppler broadening, Lamb dip spectrum, Born Oppenheimer approximation.

Module II: Microwave Spectroscopy (6 Hours)

2.1 Principal moments of inertia and classification (linear, symmetric tops, spherical tops and asymmetric tops), selection rules, intensity of rotational lines, relative population of energy levels, derivation of J_{max}, effect of isotopic substitution, calculation of intermolecular distance, spectrum of non rigid rotors.

2.2 Rotational spectra of polyatomic molecules, linear and symmetric top molecules. Stark effect and its application, nuclear spin and electron spin interaction, chemical analysis by microwave spectroscopy.

Module III: Infrared and Raman Spectroscopy (9 Hours)

3.1 Morse potential energy diagram, fundamental vibrations, overtones and hot bands, determination of force constants, diatomic vibrating rotator, break down of the Born- Oppenheimer approximation, effect of nuclearspin.

3.2 Vibrational spectra of polyatomic molecules, normal modes of vibrations, combination and difference bands, Fermi resonance. FT technique, introduction to FTIR spectroscopy. Instrumentation of FTIR

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

Module IV: Electronic Spectroscopy (9 Hours)

4.1 Term symbols of diatomic molecules, electronic spectra of diatomic molecules, selection rules, vibrational coarse structure and rotational fine structure of electronic spectrum. Franck-Condon principle, predissociation, calculation of heat of dissociation, Birge and Sponer method.

4.2 Electronic spectra of polyatomic molecules, spectra of transitions localized in a bond or group, free electron model. Different types of lasers-solid state lasers, continuous wave lasers, gas lasers and chemical laser, frequency doubling, applications of lasers.

Module V: Nuclear Magnetic Resonance Spectroscopy (18 Hours)

5.1 Theory of NMR Spectroscopy: Interaction between nuclear spin and applied magnetic field, important magnetically active nuclei. Nuclear energy levels, population of energy levels, Larmor precession, relaxation methods. Chemical shift and its representation- δ scale of PMR and CMR. Spin-spin coupling: Theory and illustration with AXsystem.

5.2 Fourier Transformation (FT) NMR Spectroscopy: Instrumentation of NMR technique, magnets, probe and probe tuning, Creating NMR signals, effect of pulses, rotating frame reference, FID, FT technique, data acquisition and storage.Pulse sequences- Pulse width, spins and magnetization vector.

5.3 Solid state NMR-Applications. Magic Angle Spinning(MAS).

Module VI: Other Magnetic Resonance Techniques (9 Hours)

6.1 EPR Spectroscopy: Electron spin in molecules, interaction with magnetic field, g factor, factors affecting g values, determination of g values ($g_{\parallel}$ and $g_{\perp}$), fine structure and hyperfine structure, Kramers' degeneracy, McConnell equation.

6.2 Theory and important applications of NQRS spectroscopy.

6.3 Mossbauer Spectroscopy: Principle, Doppler effect, recording of spectrum, chemical shift, factors determining chemical shift, application to metalcomplexes.

References

1. C.N. Banwell, E.M. McCash, Fundamentals of Molecular Spectroscopy, 4th Edn., Tata McGraw Hill,1994.
2. G. Aruldhas, Molecular Structure and Spectroscopy, Prentice Hall of India, 2001.
3. A.U. Rahman, M.I. Choudhary, Solving Problems with NMR Specroscopy, Academic Press, 1996.
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8. H. Kaur, Spectroscopy, 6thEdn.,PragatiPrakashan, 2011.
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10. D.A. McQuarrie, J.D. Simon, Physical Chemistry: A Molecular Approach, University Science Books, 1997.
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12. D.N. Sathyanarayana, Vibrational Spectroscopy: Theory and Applications, New Age International, 2007.
13. D.N. Sathyanarayana, Introduction To Magnetic Resonance

Spectroscopy ESR, NMR, NQR, IK International,2009.

Practicals - Semester I & II

INORGANIC CHEMISTRY PRACTICAL- I (PCH1CRP0122/PCH2CRP0122)

108 Hours 3 Credits

Course Outcomes

After successful completion of the course, the students should be able to

- Acquire laboratory experience in separation and identification of a mixture of metal cations
- Acquire laboratory experience in colorimetric estimation of Fe, Cu, Ni, Mn, Cr, NH_4^+, nitrate and phosphate ions
- Acquire laboratory experience in the preparation of coordination complexes
- Acquire practical knowledge in the characterization of complexes by IR and UV-Vis spectroscopy.
- Acquire synthetic skills in inorganic chemistry

Part I

Separation and identification of a mixture of four cations (a mixture of two familiar ions such as Ag^+ , Hg^{2+}, Pb^{2+}, Cu^{2+}, Bi^{2+}, Cd^{2+}, As^{3+}, $Sn^{2+,}$ Sb^{3+}, Fe^{2+}, Fe^{3+}, Al^{3+}, Cr^{3+}, Zn^{2+} , Mn^{2+},

Co^{2+}, Ni^{2+}, Ca^{2+}, Sr^{2+}, Ba^{2+}, Mg^{2+}, Li^+ , Na^+ , K^+ and $NH4^+$ and 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. Minimum eight mixtures to be given.

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.

Tris (thiourea)copper(I)complex

Potassium tris(oxalate) aluminate(III).

Hexammine cobalt (III)chloride.

Tetrammine copper (II)sulphate.

Schiff base complexes of various divalent metal ions.

Bis (dimethylglyoximato)nickel(II)

Tris (triphenylphosphine) copper(I) nitrate

Tris (acetylacetonato)iron (III)

Cis and *trans*-dichlorobis(ethylenediamine)cobalt(III) chloride

Prussianblue

References

1. A. I. Vogel, G. Svehla, Vogel's Qualitative Inorganic Analysis, 7th Edn., Longman,1996.
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, 3rdEdn., McMillian,1968.
4. V.V. Ramanujam, Inorganic Semimicro Qualitative Analysis, The National Pub.Co., 1974.
5. J. Singh, R. K. P. Singh, J. Singh, LDS Yadav, I. R. Siddiqui, J. Shrivastava, Advanced Practical Chemistry, Pragati Prakashan, 7th Edn.,2017.

ORGANIC CHEMISTRY PRACTICAL-1(PCH1CRP0222/PCH2CRP0222)

108 Hours 3 Credits

Course Outcomes

After successful completion of the course, the students should be able to

- Acquire laboratory experience in the general separation and purification of organic compounds
- Separate organic binary mixture by acid/base work-up procedures
- Perform various organic named reactions in the laboratory
- Interpret the IR and NMR spectra of the prepared compounds
- Acquire soft skills related to drawing chemical structure/reaction schemes using Chem Draw, Symyx Draw and Chem Sketch.

Part I

General methods of separation and purification of organic compounds such as:

1. Solvent Extraction
2. Soxhlet Extraction
3. Fractional Crystallization
4. TLC and Paper Chromatography
5. Column Chromatography
6. Membrane Dialysis

Part II

1. Separation of Organic binary mixtures by chemical/solvent separation methods
2. Quantitative separation of organic mixtures by column chromatography – Purity assessment of the components byTLC.

Part III

Drawing the reaction schemes (Based on Semester 1 and 2 theory) by ChemDraw, Symyx Draw and Chemsketch. Draw the structures and generate the IR and NMR spectra of the substrates and products in the following reactions:

1. Condensation
    (a) Dieckmann condensation
    (b) Claisen condensation
    (c) Darzen condensation
    (d) Aldol condensation

2. Oxidation /Reduction
    (a) Ozonolysis
    (b) Baeyer Villiger oxidation
    (c) Cannizaro reaction
    (d) Clemmenson reduction

3. Rearrangement
    (a) Benzilic acid rearrangement
    (b) Pinacol – Pinacolone rearrangement
    (c) Dienone – Phenol rearrangement
    (d) Wagner – Meerwein rearrangement

4. Pericyclic reaction
    (a) Diels – Alder reaction
    (b) Cope rearrangement

Part IV

Spectrophotometric (UV-Vis) estimations of organic compounds (eg: Nitro compounds, azo compounds etc.)

References

1. A.I. Vogel, A Textbook of Practical Organic Chemistry, Longman,1974.

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

PHYSICAL CHEMISTRY PRACTICAL-1 (PCH1CRP0322/PCH2CRP0322)

144 Hours 3 Credits

Course Outcomes

After successful completion of the course, the students should be able to

- Acquire laboratory skill in the determination of concentration of organic acids by adsorption isotherms.
- Construct phase diagrams for three component systems
- Acquire laboratory skill in calculating the composition of liquids through surface tension measurements
- Acquire practical computational chemistry knowledge in calculating vibrational frequencies, conformational energies, dipole moments etc., using modern open source computational chemistry packages.
- Acquire practical computational knowledge in the determination of Z-matrices /Cartesian coordinates of benzene and simple aromatic heterocycles.

Part A

I. Adsorption

Verification of Freundlich and Langmuir adsorption isotherm Charcoal Acetic acid or Charcoal-Oxalic acid system

Determination of concentration of given acid using the isotherm

II. Phasediagrams

Construction of phase diagram of simple eutectics

Effect of KCl/Succinic acid on Critical Solution Temperature of phenol water system

Construction of phase diagram of three component system with one pair of partially miscible liquids

III. Distribution law

Distribution coefficient of Iodine between an organic solvent and water
Determination of the equilibrium constant of the reaction $KI+I_2 \rightarrow KI_3$
Determination of unknown concentration of KI

IV. Surface tension

1. Determination of the surface tension of a liquid by
    a. Capillary rise method
    b. Drop number method
    c. Drop weight method
2. Determination of Parachor values
3. Determination of the composition of two liquids by surface tension measurements
4. Determination of CMC of surfactants by surface tension measurements

V. Heat of Solution

Determination of heat of solution from solubility measurements

Part B

VI. Computational Chemistry experiments

Experiments illustrating the capabilities of modern open source/ free computational chemistry packages in computing.

a. Single point energy
b. Geometry optimization
c. Vibrational frequencies
d. Population analysis

e. Conformational analysis of ethane, transition state search

f. Molecular orbitals, ionisation energy, electronaffinity

g. Dipolemoment, freevalence, bondorder

h. Determination of inversion barrier of simple molecules like NH_3 , H_2O,H_2O_2

i. Determination of Z-matrices /Cartesian coordinates of furan, thiophene, pyrrole and benzene using structure drawing programs like Chemsketch and wwMacMolPlt.

References

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
5. Dr. J. N. Gurtu & Amit Gurtu ADVANCED PHYSICAL CHEMISTRY EXPERIMENTS

Detailed Syllabus: Semester III

STRUCTURAL INORGANIC CHEMISTRY (PCH3CRT0122)

72 Hours 4 Credits

Course Outcomes

After successful completion of the course, the students should be able to

- Explain basic concepts associated with solids
- Compare and contrast the electrical, magnetic and optical properties of solids
- Illustrate various synthetic and structural aspects of zeolites, heteropoly acids of Mo & W, P-N, P-S compounds, B and Al compounds etc.
- Explain basics concepts of organometallic polymers
- Explain the various methods of preparation of nanoparticles, magnetic nanoparticles and thin film coating.

Module I: Solid State Chemistry (18 Hours)

1.1 Structure of solids: Imperfections in solids- line defects and plane defects. Structure of the following compounds - Zinc blende, Wurtzite, Rutile, fluorite, antifluorite, Nickel Arsenide, Perosvskite and Ilmenite. Spinels, inverse spinel structures.

1.2 Solid state reactions, diffusion coefficient, mechanisms, vacancy diffusion.Thermal decomposition of solid: Type I reactions, Type II reactions.

1.3 Phase transition in solids: Classification of phase transitions,first and second order phase transitions, martensitic transformations, order-disorder transitions and spinodal decomposition,kinetics of phase transitions, sintering, growing single crystals-crystal growth from solution, growth from melt and vapour deposition technique.

Module II: Electrical, Magnetic and Optical Properties (18 Hours)

2.1 Free electron theory of solids. Band theory of solids: Applications to Transition metal compounds and compounds like NaCl, MgO and fullerenes. Energy bands-conductors and non-conductors, Mechanism of intrinsic and extrinsic semiconductors. Mobility of charge carriers- Hall Effect (derivation required). Piezo electricity, pyroelectricity and ferro electricity- hysteresis.

2.2 Magnetic properties of transition metal oxides, garnets, spinels, ilmenites and perovskites, magnetoplumbites. Photoconductivity, photovoltaic effects, luminescence, applications of optical properties-phosphors, solid state lasers and solar cells.

2.3 Conductivity of pure metals. Super conductivity-Type I and Type II superconductors, Meisner effect, BCS theory of superconductivity (derivation not required)-Cooper pairs. High temperature superconductors, super conducting cuprates - YBaCu oxide system. Josephson's Junction, conventional superconductors, organic superconductors, fullerenes, carbon nanotubes and graphenes.

Module III: Inorganic Chains, Rings, Cages and Clusters (18 Hours)

3.1 Chains: Catenation, heterocatenation, silicones. Zeolites: Synthesis, structure and applications, isopoly acids of vanadium, molybdenum and tungsten, heteropoly acids of Mo and W, polythiazil-one dimensional conductors. Infinite metalchains

3.2 Rings: Topological approach to boron hydrides, styx numbers. 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 phosphorouscompounds.

3.3 Cages and Clusters: Synthesis, structure and bonding of cage like structures of phosphorous. Boron cage, - Boranes and carboranes, - Wade-Mingos rule, aluminium, indium and gallium clusters, cages and clusters of germanium, tin and lead, cages and clusters of tellurium, Mercuride clusters in amalgams. Medical applications of boron clusters- nucleic acid precursors, DNA binders, application of C_2B_{10} for Drug Design, Nuclear receptor ligands bearing C_2B_{10}cages.

Module IV: Organometallic Polymers (9 Hours)

5.1 Polymers with organometallic moieties as pendant groups, polymers with organometallic moieties in the main chain, condensation polymers based on ferrocene and on rigid rod polyynes, poly(ferrocenylsilane)s, applications of Poly(ferrocenylsilane)s and related polymers, applications of rigid-rod polyynes, polygermanes and polystannanes, polymers prepared by ring opening polymerization, organometallic dendrimers.

Module V: Nanomaterials and their Applications (9 Hours)

6.1 General strategies for synthesis of nanomaterials. Mechanical, electronic, optical and magnetic properties and applications of nanomaterials.

6.2 Preparation of thin films, electrochemical methods, chemical vapour deposition, indium tin oxide and their coatings.

6.3 Two dimensional nano materials with special emphasis on graphene, borophene.

6.4 Magnetic Resonance Imaging (MRI) and Contrast Enhancement using magnetic nanoparticles, biomedical applications of magnetic nanoparticles.

References

1. L.V. Azaroff, Introduction to Solids, Mc Graw Hill,1984.
2. A.R. West, Solid State Chemistry and its Applications, Wiley-India, 2007.
3. D.K. Chakrabarty, Solid State Chemistry, New Age Pub., 2010.
4. D.M. Adams, Inorganic Solids: An Introduction to Concepts in Solid State Structural Chemistry, Wiley,1974.
5. C.N.R. Rao, K.J. Rao, Phase Transitions in Solids, McGraw Hill, 2010.
6. B.E. Douglas, D.H. McDaniel, J.J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Edn., John Wiley & sons, 2006.
7. Earnshaw, Introduction to Magnetochemistry, Academic Press,1968.
8. J.E. Huheey, E.A. Keiter, R.L. Keiter, Inorganic Chemistry Principles of Structure and Reactivity, 4thEdn., Harper Collins CollegePub.,1993.
9. F.A. Cotton, G. Wilkinson, C.A. Murillo, M. Bochmann, Advanced Inorganic Chemistry, 6thEdn.,Wiley-Interscience,1999.

10. K.F. Purcell, J.C. Kotz, Inorganic Chemistry, Holt-Saunders,1977.
11. Wai Kee Li, Gong-Du Zhou, homas Chung Wai Mak, Advanced Structural Inorganic Chemistry, International Union of Crystallography,2008.
12. Matthias Driess, Heinrich Nӧth, Molecular Clusters of the Main Group Elements, Wiley-VCH, 2004.
13. Richard J.D. Tilley, Understanding Solids, 2nd edition, Wiley, 2013.
14. G.L. Hornyak, J.J. Moore, H.F. Tibbals, J. Dutta, Fundamentals of Nanotechnology, CRC Press, 2009.
15. Chris Binns, Introduction to nanoscience and nanotechnology, wiley, 2010.
16. Vadapalli Chandrasekhar, Inorganic and organometallic polymers, Springer, 2005.
17. Anthony R. West, Basic Solid State Chemistry, John Wiley and Sons,1988.
18. F. Cesano, D. Scarano, Graphene and Other 2D Layered Nanomaterial-Based Films: Synthesis, Properties and Applications, Mdpi AG, 2019.

ORGANIC SYNTHESES (PCH3CRT0222)

72 Hours 4 Credit

Course Outcomes

After successful completion of the course, the students should be able to

- Recognize the use of various oxidation and reduction agents in organic chemistry and apply them suitably
- Relateand analyze modern synthetic methods of formation of C-C and C-Heteroatom bonds
- Apply synthetic chemistry for the construction of carbocyclic and heterocyclic compounds
- Understand and apply suitably various protecting groups in organic synthesis
- Analyze the research methodology of chemistry

Module I: Organic Synthesis via Oxidation and Reduction (18 Hours)

1.1 Oxidation reactions: Metal based and non-metal based oxidations of (a) alcohols to carbonyls [(Chromium-John's oxidation, Collin's oxidation, Sarrett oxidation), Manganese, aluminium (Oppenauer oxidation) and DMSO(Swern oxidation, Moffatt–Pfitzner oxidation, Kornblum oxidation, Corey-Kim oxidation)] based reagents (b) alkenes to epoxides (peroxides/peracids based)-Sharpless asymmetric epoxidation, Jacobsen epoxidation, Shi epoxidation (c) alkenes to diols (Manganese and Osmium based)- Prevost reaction and Woodward modification (d) alkenes to carbonyls with bond cleavage (Manganese based, ozonolysis) (e) alkenes to alcohols/carbonyls without bond cleavage-hydroboration-oxidation, Wacker oxidation, selenium based allylic oxidation (f) ketones to ester/lactones- Baeyer-Villigeroxidation.

1.2 Reduction reactions: (a) Catalytic hydrogenation (Heterogeneous: Palladium/Platinum/Rhodium and Nickel. Homogeneous: Wilkinson). (b) Metal based reductions- Birch reduction, pinacol formation, acyloin formation, MPV reduction (c) Enzymatic reduction using Baker's yeast.

Module II: Modern Synthetic Methods (18 Hours)

2.1 Baylis-Hillman reaction, Henry reaction, Nef reaction, Kulinkovich reaction, Ritter reaction, Sakurai reaction, Tishchenko reaction. Brook rearrangement. Tebbe olefination. Metal mediated C-C and C-X coupling reactions: Heck, Stille, Suzuki-Miyaura, Negishi, Sonogashira, Nozaki-Hiyama-Kishi, Buchwald-Hartwig, Ullmann and Glaser coupling reactions. Click reactions (Huisgen 1,3-dipolaraddition).

2.2 Multi component reactions-Ugi reaction, Passerini reaction and Biginelli reaction.

Module III: Synthetic Reagents (9 Hours)

3.1 Hydride transfer reagents from Group III and Group IV in reductions - $LiAlH_4$, DIBAL-H, Red-Al, $NaBH_4$ and $NaCNBH_3$, selectrides, trialkylsilanes and trialkyl stannane. Aluminum isopropoxide (oxidation and reduction).Reagents such as NBS, DDQ and DCC.Gilmann reagent. DMAP-Borane, PCC, DEAD (Mitsunobureaction).

Module IV: Construction of Carbocyclic and Heterocyclic Ring Systems (9 Hours)

4.1 Synthesis of four, five and six-membered rings, photochemical approaches for the synthesis of four membered rings-oxetanes and cyclobutanes, ketene cycloaddition (inter and intra molecular), Pauson-Khand reaction, Volhardt reaction, Bergman cyclization, Nazarov cyclization, cation-olefin cyclization and radical-olefin cyclization.

4.2 Inter-conversion of ring systems (contraction and expansion)-Demjenov reaction, Reformatsky reaction. Construction of macrocyclic rings-ring closing metathesis (Grubb's catalyst).

4.3 Formation of heterocyclic rings: 5-membered ring heterocyclic compounds with one or more than one hetero atom like N, S or O - pyrrole, furan, thiophene, imidazole, thiazole and oxazole.

Module V: Protecting Group Chemistry (9 Hours)

5.1 Protection and deprotection of hydroxy, carboxyl, carbonyl, and amino groups. Chemo and regio selective protection and deprotection.

5.2 Protection and deprotection in peptide synthesis: common protecting groups used in peptide synthesis, protecting groups used in solution phase and solid phase peptide synthesis (SPPS).

Module VI: Research Methodology of Chemistry (9 Hours)

6.1 Types of research: Fundamental, applied, historical and experimental research.

6.2 Chemical literature: Primary, secondary and tertiary sources of literature. Classical and comprehensive reference. Literature databases: Science Direct, SciFinder.

6.3 Scientific writing: Research reports, thesis, journal articles, books. Types of publications: articles, communications, reviews.

6.4 Important scientific and Chemistry Journals, Impact factor, reputation of journals

6.5 Journal Club *(As an assignment/Seminar – Students refer recent articles published in reputed science (chemistry) journals and present in front of the teacher(s) and students).*

References

1. M.B. Smith, Organic Synthesis, 3rd Edn., Wavefunction Inc., 2010.
2. F.A. Carey, R. I. Sundberg, Advanced Organic Chemistry, Part A and B, 5th Edn., Springer, 2007.
3. Ojima, Catalytic Asymmetric Synthesis, 3rd Edn., John Wiley & Sons,2010.
4. W. Carruthers, I. Coldham, Modern Methods of Organic Synthesis, 4th Edn., Cambridge University Press,2004.
5. J. Clayden, N. Greeves, S. Warren,P. Wothers, Organic Chemistry, Oxford Univsity Press, 2001.

6. R. Noyori, Asymmetric Catalysis in Organic Synthesis, John Wiley & Sons,1994.
7. L. Kuerti, B. Czako, Strategic Applications of Named Reactions in Organic Synthesis, Elsevier Academic Press, 2005.
8. R.O.C. Norman, J.M. Coxon, Principles of Organic Synthesis, 3rd Edn., Chapmann and Hall,1993.
9. V.K. Ahluwalia, L.S. Kumar, S. Kumar, Chemistry of Natural Products, CRS Press, 2007.
10. R.L. Dominoswki, Research Methods, Prentice Hall,1981.
11. J.W. Best, J.V. Kahn, Research in Education, 10th Edn., Pearson/Allyn & Bacon, 2006.
12. H. F. Ebel, C. Bliefert, W. E. Russey: The Art of Scientific Writing: From Student Reports to Professional Publications in Chemistry and Related Fields, VCH, Weinheim, New York 1987.

CHEMICAL KINETICS, SURFACE CHEMISTRY AND CRYSTALLOGRAPHY

(PCH3CRT0322)

72 Hours 4 Credits

Course Outcomes

After successful completion of the course, the students should be able to

- Learn the advanced aspects of chemical kinetics
- Recognize various factors those affect the kinetics of reactions
- Learn the kinetic aspects of surface chemistry
- Explain the basic concepts of crystallography
- Acquire basic understanding of single crystal X-ray crystallography and recognize its application

Module I: Chemical Kinetics (27 Hours)

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

1.2 Unimolecular reactions: Lindemann- Hinshelwood mechanism, qualitative idea of RRKM theory.

1.3 Chain reactions: Chain initiation processes, steady state treatment, kinetics of H_2-Cl_2 and H_2-Br_2 reactions, Rice-Herzfeld mechanism for decomposition of ethane and acetaldehyde, Goldfingr-Letort-Niclause rules, branching chains, Semenov- Hinshelwood mechanism of branching chains, upper and lower explosion limits, the H_2-O_2 reaction, kinetics of step growth, free radical, cationic and anionic polymerization reactions.

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

1.5 Reactions in solution: Factors determining reaction rates in solutions, effect of dielectric constant and ionic strength, cage effect, Bronsted-Bjerrum equation, primary and secondary kinetic salt effect.

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

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

1.8 Introduction to oscillating chemical reactions: autocatalysis, autocatalytic mechanism of oscillating reactions, the Lotka-Volterra mechanism, the brusselator, the oreganator, bi stability.

Module II: 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 Application of low energy electron diffraction and photoelectron spectroscopy, ESCA and Auger electron spectroscopy, scanning probe microscopy-AFM and STM, ion scattering, SEM and TEM in the study of surfaces.

2.3 Surface Enhanced Raman Scattering, surfaces for SERS studies, chemical enhancement mechanism, surface selection rules, principle and application of SERS in surface chemistry.

2.4 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, the Eley-Rideal mechanism and the Langmuir-Hinshelwood mechanism, flash desorption.

2.5 Colloids: structure and stability, the electrical double layer, zeta potential, electrokinetic phenomena-sedimentation potential and streaming potential, Donnan membrane equilibrium.

2.6 Macromolecules: Different averages, methods of molecular mass determination - osmotic, viscosity, sedimentation and light scatteringmethods.

Module III: Crystallography (18 Hours)

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

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

3.3 Liquid crystals: Mesomorphic state, types, examples and application of liquid crystals.

References

1. J. Rajaram, J.C. Kuriakose, Kinetics and Mechanisms of Chemical Transformations, Macmillan India, 2000.
2. K.J. Laidler, Chemical kinetics, 3rd Edn., Harper & Row,1987.
3. Kalidas, Chemical Kinetic Methods: Principles of Fast Reaction Techniques and Applications, New Age International,2005.
4. J.W. Moore, R.G. Pearson, Kinetics and Mechanisms, John Wiley & Sons, 1981.
5. P.W. Atkins, Physical Chemistry, 9th Edn, Oxford University press,2010
6. D.A. McQuarrie, J.D. Simon, Physiacl chemistry: A Molecular Approach,University Science Books,1997
7. A.W. Adamson, A.P. Gast, Physical Chemistry of Surfaces, 6thEdn., John Wiley & sons,1997.

8. L.V. Azaroff, Introduction to Solids, Mc Graw Hill, 1984.
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11. Charles Kittel, Introduction to Solid State Physics 8th edition.
12. Yoshio Waseda-Eiichiro Matsubara, Kozo Shinoda, X-Ray Diffraction Crystallography Introduction, Examples and Solved Problems
13. Christopher Hammond , The Basics of Crystallography and Diffraction 3rd edition

SPECTROSCOPIC METHODS IN CHEMISTRY (PCH3CRT0422)

54 Hours 4 Credits

Course Outcomes

After successful completion of the course, the students should be able to

- Apply UV-Vis spectroscopy to compare various organic compounds
- Apply IR spectroscopy to compare various organic compounds and to recognize various functional groups present in them.
- Apply ^{1}H &^{13}C NMR spectroscopy for the elucidation of the structure of of organic compounds
- Explain various aspects of mass spectroscopy and apply it in finding the fragments present/atoms present in organic compounds
- Acquire skill in elucidating the structure of organic compounds using IR, NMR, mass and UV-Vis spectroscopy

Module I: Ultraviolet-Visible and Chiro-optical Spectroscopy (9 Hours)

1.1 Energy levels and selection rules, Woodward-Fieser and Fieser-Kuhn rules.

1.2 Influence of substituent, ring size and strain on spectral characteristics. Solvent effect, Stereochemical effect, non-conjugated interactions. Chiro-optical properties-ORD, CD, octant rule, axial haloketone rule, Cotton effect-applications.

1.3 Problems based on the above topics.

Module II: Infrared Spectroscopy (9 Hours)

2.1 Fundamental vibrations, characteristic regions of the spectrum (finger print and functional group regions), influence of substituent, ring size, hydrogen bonding, vibrational coupling and field effect on frequency, determination of stereochemistry by IR technique.

2.2 IR spectra of C=C bonds (olefins and arenes) and C=Obonds.

2.3 Problems on spectral interpretation with examples.

Module III: Nuclear Magnetic Resonance Spectroscopy (18 Hours)

3.1 Magnetic nuclei with special reference to ^1H 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. ^1H 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, Pascal's triangle, coupling constant, mechanism of coupling- Dirac model. Karplus curve, quadrupole broadening and decoupling, homotopic, enantiotopic and diastereotopic protons, virtual coupling, long range coupling. NOE and crosspolarization.

3.3 Simplification non-first order spectra to first order spectra: shift reagents, spin decoupling and double resonance, off resonance decoupling. Chemical shifts and homonuclear/heteronuclear couplings. Basis of heteronuclear decoupling.

3.4 2D NMR and COSY, HOMOCOSY and HETEROCOSY

3.5 Polarization transfer, selective population inversion, DEPT., sensitivity enhancement and spectral editing, MRI.

3.6 Problems on spectral interpretation with examples

Module IV: Mass Spectrometry (9 Hours)

4.1 Molecular ion: Ion production methods (EI). Soft ionization methods: SIMS, FAB, CA, MALDI-TOF, PD, field desorption electrospray ionization,fragmentation patterns (polyenes, alkyl halides, alcohols, phenols, aldehydes and ketones, esters),nitrogen and ring rules, McLafferty rearrangement and its applications, HRMS, MS-MS, LC-MS,GC-MS.

4.2 Problems on spectral interpretation withexamples.

Module V: Structural Elucidation Using SpectroscopicTechniques (9 Hours)

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

References

1. D.L. Pavia, G.M. Lampman, G.S. Kriz, Introduction to Spectroscopy, 3rd Edn., Brooks Cole,2000.
2. A.U. Rahman, M.I. Choudhary, Solving Problems with NMR Specroscopy, Academic Press,1996.
3. L. D. Field, S. Sternhell, J. R. Kalman, Organic Structures from Spectra, 4th Edn., John Wiley & sons,2007.
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9. W. Kemp, Organic Spectroscopy, 2nd Edn., Macmillan,1987.
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11. E.B. Wilson Jr., J.C. Decius, P.C. Cross, Molecular Vibrations: The Theory of Infrared and Raman Vibrational Spectra, Dover Pub.,1980.
12. Online spectral databases including RIO-DB.

Detailed Syllabus: Semester IV

Elective Group A

ADVANCED INORGANIC CHEMISTRY (PCH4CRT0122)

90 Hours 4 Credits

Course Outcomes

After successful completion of the course, the students should be able to

- Apply group theory to coordination complexes
- Learn various inorganic spectroscopic methods and apply them suitably
- Illustrate the various concepts associated with the photochemistry of coordination complexes
- Understand various techniques of preparation, characterization, properties and uses of various inorganic materials including nano materials and metal organic frameworks
- Acquire knowledge in the fundamental aspects with regard to unconventional approaches towards the activation of small molecules and hydrogenation reactions.

Module I: 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- ferrocene, formation of symmetry adapted group of ligand, MO diagrams.

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, splitting terms for orbitals, energy levels, d-d transition-selection rules. Determination of modes of vibrations in IR and Raman spectra using character tables in tetrahedral, octahedral and square planar complexes.

Module II: Inorganic Spectroscopic Methods (9 Hours)

2.1 Infrared Spectroscopy: Structural elucidation of coordination compounds containing the following molecules/ions as ligands - NH_3, PR_3, H, H_2, ethylene, H_2O, CO, NO, CN^-, OH^-, SO_4^{2-}, NO_2^- and X^- (X=halogen).

2.2 ^{1}H NMR of transition metal complexes containing H and H_2 as ligands, ^{31}P NMR of transition metal phosphine complexes, ^{19}F NMR and coupling with ^{13}C.

2.3 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, electron-electron interactions, multiple resonance.

Module III: Inorganic Photochemistry (9 Hours)

3.1 Excited states in transition metal complexes: Intra-ligand excited states and metal-centred excited states.Photochemical reactions: Substitution and redox reactionsof Cr(III), Co(III), Rh(III) and Ru(II) complexes, manganese-based photosystems for the conversion of water into oxygen, chemical actinometry and photochromism, metal-metal multiple bonds, dissociative photochemistry, ligandloss.

3.2 Metal complex sensitizers, electron relay, semiconductor supported metal oxide systems, water photolysis, nitrogen fixation and CO_2 reduction, dinitrogen splitting.

Module IV: Nanomaterials (18 Hours)

4.1 Inorganic nanomaterials: General introduction to nanomaterials,synthesis and applications of nanoparticles of gold, silver, rhodium, palladium and platinum,synthesis and applications of metal oxides of transition and non-transition elements-SiO_2, TiO_2, ZnO, Al_2O_3, iron oxides and mixed metal oxide nanomaterials, non-oxide inorganic nanomaterials, porous silicon nanomaterials-fabrication and chemical and biological sensing applications.

4.2 Characterisation of Nanomaterials: UV-visible, Raman, XRD, SEM, TEM and AFM techniques.

4.3 Diversity in nanosystems: Self-assembled monolayers on gold-growth process and phase transition, gas phase clusters-formation, detection and analysis, quantum dots- preparation, characterization and applications, nanoshells-types ofsystems, characterization and application, inorganic nanotubes-synthetic strategies, structures, properties and applications. Nanocomposites- natural nanocomposites, polymer nano composites, metal and ceramic nano composites and clay nano composites.

4.4 Evolving interfaces of nanotechnology: Nano biotechnology, nano-biosensors, nanotechnology for manipulation of biomolecules- optical tweezers, dielectrophoresis, biochips, labs on chips, and integrated systems, nanocatalysts, nanomedicines- importance of nanomaterials in the pharmaceutical industry and future possibilities for medical nanotechnology, nanoparticles for medical imaging, nano particles for targeting cancer cells, nanoencapsulation for drug delivery to tumours.

Module V: Chemistry of Materials (9 Hours)

5.1 Ceramic Structures:Mechanical properties, clay products, refractories-characterisation, properties and applications, non-silicon semiconductors as light emitting diodes, thermoelectric (TE) materials, applications of metals and alloys in hydrogen storage, inorganic organic hybrid composites- sol-gel ceramics, fillers in elastomers, polymer-modified ceramics.

5.2 Synthetic strategies for inorganic material design: Direct Combination, low temperature techniques, combinatorial synthesis.

Module VI: Metal Organic Frame Works (9 Hours)

6.1 Introduction, porous coordination polymers, frameworks with high surface area, Lewis acid frameworks, soft porous crystals, design of metal organic frameworks and design of functional metal organic frameworks by post-synthetic modification.

6.2 Applications of metal organic frameworks- separation and purification of gases by MOFs, hydrogen storage, MOFs in the pharmaceutical world.

Module VII: Unconventional Activation of Small Molecules (9 Hours)

7.1 Dihydrogen splitting and hydrogenation of olefins and polar substrates like ketones and imines: Concerted and Stepwise activation–Noyori's metal-ligand bifunctional hydrogenation – Shvo catalyst – Milstein's aromatization-dearomatization strategy, ionic hydrogenation, transfer hydrogenations of ketones and imines.

7.2 Frustrated Lewis Pairs (FLPs): B-P and B-N adducts – activation of H_2 and CO_2 – hydrogenation of aklynes, ketones, imines and nitriles.

7.3 Ammonia borane: Application in hydrogenation – H_2 storage .

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ADVANCED ORGANIC CHEMISTRY(PCH4CRT0222)

90 Hours 4 Credits

Course Outcomes

After successful completion of the course, students should be able to

- Explain the concepts of molecular recognition and organic supramolecular chemistry
- Recognize alternative green methods adopted in organic synthesis
- Apply synthetic knowledge in bioorganic chemistry, medicinal chemistry and natural product chemistry
- Recognize various well known stereoselective syntheses and understand their strategies of asymmetric induction.
- Apply retrosynthetic strategy for the preparation of complex organic molecules

Module I: Supramolecular Chemistry and advanced polymer chemistry (18 Hours)

1.1 Introduction to supramolecular chemistry: Host, Guest, Host-Guest complex, Lock and key principle, Pre-organisation, Complementarity.

1.2 Molecular recognition, forces involved in molecularrecognition.

1.3 Cation binding Hosts: Crown ethers, Cryptands and Calixarenes

1.4 Anion binding hosts: Cyclophanes and Cyclodextrins.

1.5 Basic ideas in Molecular clefts, tweezers, macrocyclic polyamines and Siderophores.

1.6 Conducting polymers, temperature resistant and flame retardant polymers

1.7 Dendrimers and dendritic polymers: Terminology, classification of dendrimers. Methods of synthesis: convergent and divergent approaches, applications of dendrimers. Hyperbranched polymers: Definition, synthesis, applications.

Module II: Green Alternatives to Organic Synthesis (9 Hours)

2.1 Introduction to Green Chemistry, atom economy

2.2 Twelve principles of Green Chemistry, how to plan a green synthesis.

2.3 Green Solvents: Ionic liquids, supercritical CO_2, fluorous solvents,PEG

2.4 Microwave assisted organic synthesis: Principle, example.

2.5 Sonochemical synthesis : Principle,example

2.6 Green alternatives to organic synthesis: Thiamine catalyzed benzoin condensation, Montmorillonite K-10 catalysed Pinacol-Pinacolone rearrangement, photochemical reduction of benzophenone to benzopinacol, synthesis of adipic acid from cyclohexene, synthesis of Ibuprofen.

Module III: Biosynthesis and Biomimetic Synthesis (9 Hours)

3.1 Basic principles of the biosynthesis of terpenes, steroids, alkaloids, carbohydrates, proteins and nucleic acids, biosynthesis of cholesterol, α-terpineol, morphine, glucose and phenyl alanine, biogenesis of isoprenoids and alkaloids, biomimetic synthesis of progesterone (Johnson synthesis).

Module IV:Stereoselective Transformations (9 Hours)

4.1 Assymmetric induction - chiral auxiliaries and chiral pool.

4.2 Enantioselective catalytic hydrogenation developed by Noyori and Knowels.

4.3 Assymetric aldol condensation pioneered by Evans.

4.4 Assymmetric Diels-Alder reactions.

4.5 Enatioseletive synthesis of Corey lactone

Module V: Chemistry of Natural Products and Biomolecules (18 Hours)

5.1 Synthesis of camphor, atropine, papaverine, quinine, quercetin, β-carotene, biosynthesis of PGE2 and PGF2α.

5.2 Carbohydrates: Structure of monosacharides (glucose, fructose), disachrides (maltose, sucrose and cellobiose), polysachrides (starch and cellulose)

5.3 Structure of proteins and nucleic acids, methods for primary structure determination of peptides (N-terminal - Sanger's method and Edmond's method; C-terminal - Akabora method and carboxy peptidase method), replication of DNA, protein biosynthesis, DNA sequencing, DNA profiling and the Polymerase Chain Reaction(PCR).

Module VI: Medicinal Chemistry and Drug Designing (9 Hours)

6.1 Introduction to Drug design: Modelling techniques, receptor proteins, drug-receptor interaction, drug action, drug selectivity, drug metabolism (Phase I and Phase II).

6.2 Mode of action of Warfarin (anti coagulant), organic nitrates (anti-anginal drug), Captoril (anti hypertensive agent), Chloroquin (antimalarial drug).

6.3 Antibiotics: Penicillins (SAR expected), mode of action of chloramphenicol, tetracyclins and cephalosporins, drugs for cancer (Methotrexate), AIDS (Zidovudin) and diabetes (Metformin).

Module VII: Advances in Polymer Chemistry (9 Hours)

7.1 Organic Conducting polymers-preparation and applications, conducting mechanisms, polyaniline, polyacetylene, polyparaphenylene and polypyrrole. Polymers and their biomedical applications. Flame retardant polymers.

7.2 Organic dendrimers and dendritic polymers: Terminology, classification of dendrimers. Methods of synthesis: convergent and divergent approaches, applications of dendrimers. Hyper branched polymers: Definition, synthesis, applications.

Module VIII:Retrosynthetic Analysis (9 Hours)

8.1 Basic principles and terminology of retrosynthesis: synthesis of aromatic compounds, one group and two group C-X disconnections; one group C-C and two group C-C disconnections.

8.2 Amine and alkene synthesis: important strategies of retrosynthesis, functional group transposition, important functional group interconversions. Retrosynthesis of D- luciferin. Functional equivalents and reactivity-Umpolung reaction (Ireland-Claisen rearrangement).

References

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ADVANCED PHYSICAL CHEMISTRY (PCH4CRT0322)

90 Hours 4 Credits

Course Outcomes

After the successful completion of the course, students should be able to

- Explain advanced concepts in the photochemistry of molecules
- Illustrate the basics of various diffraction techniques like neutron diffraction, X-ray, AAS, AES, FES etc.
- Learn advanced electrochemistry and apply it to solve various electrochemical problems
- Compare and contrast various electroanalytical techniques
- Explainthe concepts associated with advanced thermodynamics particularly of biological processes.

Module I: Photochemistry (18 Hours)

1.1 Quantum yield, chemical actinometry, excimers and exciplexes, photosensitization, chemiluminescence, bioluminescence, thermoluminescence, pulse radiolysis, hydrated electrons, photostationary state, dimerization of anthracene, ozone layer in the atmosphere.

1.2 Principle of utilization of solar energy: solar cells, types of solar cells-amorphous silicon solar cell, cadmium telluride solar cell, copper indium gallium selinide solar cell.

1.3 Quenching of fluorescence and its kinetics, Stern-Volmer equation, concentration quenching, fluorescence and structure, delayed fluorescence, E-type and P-type, effect of temperature on emissions, photochemistry of environment, green house effect, two photon absorption spectroscopy, lasers in photochemical kinetics.

Module II: Fluorescence Spectroscopy (9 Hours)

2.1 Instrumentation: light source, monochromator, optical filters, photomultiplier tube, polarizers, fluorescence sensing, mechanism of sensing, sensing techniques based on collisional quenching, energy transfer and electron transfer, examples of pH sensors. Novel fluorephores: long life time metal-ligand complexes.

Module III: Diffraction Methods and Atomic Spectroscopic Techniques (9 Hours)

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

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

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

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

Module IV: Electrochemistry and Electromotive Force (27 Hours)

4.1 Theories of ions in solution, Drude and Nernst's electrostriction model and Born's model, Debye-Huckel theory, derivation of Debye-Huckel-Onsager equation, validity of DHO equation for aqueous and non aqueous solutions, Debye-Falkenhagen effect, conductance with high potential gradients, activity and activity coefficients in electrolytic solutions, ionic strength, Debye-Huckel limiting law and its various forms, qualitative and quantitative tests of Debye-Huckel limiting equation, deviations from the DHLL, ion association, triple ions and conductance minima.

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, electro capillary, Lippmann equation, membrane potential.

4.3 Fuel cells - Theory and working of fuel cells- methanol fuel cell, H_2-O_2 fuel cell and solid oxide fuel cells.

4.4 Solubilty product principle, solubility in presence of common ion, activity coefficient and solubility measurements, determination of activity coefficient from equilibrium constant measurements.

4.5 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.

Module V: 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.

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

5.4 Amperometric titrations: General principles of amperometry, instrumentation, application of amperometry in the qualitative analysis of anions and cations in solution, merits and demerits of amperometric titrations.

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

Module VI: Advanced Thermodynamics (9 Hours)

6.1 Thermodynamics of irreversible processes with simple examples, general theory of non-equilibrium processes, entropy production, the phenomenological relations, the principle of microscopic reversibility, Onsager reciprocal relations, thermal osmosis and thermo electric phenomena.

6.2 Bioenergetics, coupled reactions, ATP and its role in bioenergetics, high energy bond, free energy and entropy change in ATP hydrolysis, thermodynamic aspects of metabolism and respiration, glycolysis, biological redox reactions.

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Elective Group B

ADVANCES IN POLYMER SCIENCE AND TECHNOLOGY (PCH4CRT0422)

Credit: 4 Contact Lecture Hours: 90

Course Outcomes

- To have a well organised knowledge about speciality polymers,polymer blends and composites, polymer mixing and compounding, adhesives, techniques of surface coating
- To acquire knowledge about fibre science and technology
- To Study the, methods of measuring the molecular weight, polymerization kinetics and Copolymerization and polymer processing technologies.
- To understand about the techniques of polymer analysis
- To study mechanical properties and applications of polymers

Module I: Speciality Polymers (18 Hours)

1.1 Poly electrolytes-the water soluble charged polymers, ionomers (ion containing polymers, conducting polymers, solid polymer electrolytes (SPE), electroluminescent polymers, fluoropolymers, block copolymers(multiphase polymers), polymer colloids, thermoplastic elastomers(TPE), polyblends (heterogeneous plastics), inter penetrating network (IPN) polymers, thermally stable polymers, telechelic polymers (functional polymers) polymer microgel, biomedical polymers.

1.2. Liquid crystalline polymers: definition and synthesis, main chain liquid crystalline polymers, side chain liquid crystalline polymers, combined side chain- main chain liquid crystalline polymers, liquid crystalline polymer networks, liquid crystalline elastomers, application of liquid crystalline polymers.

1.3. Dendritic polymers: origin of dendrimers, structure, properties, design and synthesis- divergent growth method, convergent growth method, medicinal application.

1.4. Introduction to: polymers for organic light-emitting diodes (OLEDs), organic and hybrid solar cell, supramolecular polymer science.

Module II: Adhesives and Surface Coating (12 Hours)

2.1. Adhesives: introduction, theory, surface treatment, joint design, physical nature of adhesives, types of adhesives, natural glues, applications, elastomer adhesives, synthetic adhesives, olefinic polymer adhesives, types of epoxy adhesives, inorganic adhesives, bio adhesives, test methods in determining the strength and properties of adhesives.

2.2. Surface coating: introduction, types of coating, drying oils, types of resins, surfactants, surface preparation, coating methods, solvent selection, methods of coating, theory of powder coating, application of powder coating, curving process.

2.3. Corrosion, electroplating, hazards and safety measures in paint industry.

Module III: Polymer Blends and Composites (18 Hours)

3.1. Polymer blends: classification, principles and methods involved in the preparation of different polymer blends, study of polymer blends and alloys on the basis of miscibility, criteria for selection of polymer.

3.2 Compatibility of blends: principles of solubility and compatibility, thermodynamics of miscibility, mechanical compatibility.

3.3 Phase morphology: phase separation behaviour, morphology of blends and its determination- electron microscopy- domain structure.

3.4. Introduction to rheology of polymer blends: its relevance in processing, rheology–phase morphology relationships and their relevance, micro rheology, rheological models-solution, and suspension models.

3.5. Industrial applications of polymer blends.

3.6. Polymer composites: fundamental concepts, factors influencing the performance of polymer composites-aspect ratio, void content, length of the fibre, nature of the fibre, structure property relationship between fibre and matrix, modifications of the fibre surface, degree of interaction between fibre and matrix, wetting behaviour, degree of cross linking etc.,

3.7 Processing of thermoplastic composites- types of processing methods, solution, film, lamination, sandwitch etc., processing conditions, advantages and disadvantages.

3.8. Fabrications of thermoset composites: hand layup method, compression and transfer moulding, pressure and vacuum bag process, filament winding, protrusion, reinforced RIM, RRIM, injection moulding of thermosets, SMC and DMC, advantages and disadvantages of each method.

3.9. Nano-composites- definition, types, methods of fabrication, characterization, uses and applications.

Module IV: Polymer Compounding and Processing (18 Hours)

4.1. Polymer mixing: introduction, basic concepts, mechanism of mixing and dispersion, mixing of solid-solid, liquid-liquid and liquid-solid, dispersive mixing, distributive mixing and laminar mixing, mixing indices, scale of segregation and intensity of segregation, kinetics of mixing, rheology of filled polymers.

4.2. Compounding: introduction, types and characteristics of compounds-polymer blends, polymer formulations, filled polymers and polymer composites, compounding practice, mixing types, solid additives, morphology of filler additives, filler reinforcement, compatibilizers-mechanism and theory, filler surface modification and interfacial agents, dispersion of polymer nanoparticles in polymer melt, fillers and reinforcements viz. carbon black, ZnO, calcium carbonate, titanium oxide, nano clay, glass fibers, organic fillers, nanofillers.

4.3. Polymer processing: casting-die casting, rotational casting, film casting, thermoforming, foaming, lamination, reinforcing, processing of fibres-dry spinning, wet spinning, melt spinning, moulding processes-compression moulding, injection moulding, transfer moulding, blow moulding, extrusion moulding, calendaring.

Module V: Fibre Science and Technology (12 Hours)

5.1. Basic concepts, structural attributes of fibres, Fibre characteristics

5.2. Natural fibres: natural fibres of vegetable origin, the seed and fruit fibres, natural fibres of animal origin-silk, natural mineral fibre

5.3. Man-made fibres: introduction, spinning, semi-synthetic fibres from cellulose, regenerated protein fibres, synthetic fibres-rayon, polyethylene terephthalate, nylon 6 and nylon 66, acrylics, polyolefins, polyvinyl chloride, polyvinyl alcohol.

5.4. Miscellaneous fibres -carbon fibre, glass fibre, boron fibre, ceramic fibre-alumina fibre.

5.5. Brief outline of manufacture of textiles: fibres to yarn, yarns to fabrics-weaving, knitting, braiding, compound fabric constructions, finishing processes, dyeing and printing.

Module VI: Latex Technology (12 Hours)

6.1. Natural rubber latex: composition of latex, conservation, gelation, stability of latex & flocking, chemical modifications of natural latex - prevulcanisation, grafting, halogenations, hydro halogenations.

6.2. Synthetic latex: SBR lattices and its types like XSBR, properties, NBR lattices and its types and properties, poly chloroprene and its properties, butyl lattices, comparative study of natural, SBR, NBR & poly chloroprene.

6.3. Latex testing: sampling, total solids, dry rubber content, pH, VFA number, KOH number, mechanical & chemical stability.

6.4. Manufacturing techniques: dipping-principle & process, foam making-principle, dunlop process, talalay process.

References

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ANALYTICAL CHEMISTRY (PCH4CRT0522)

Credit: 4 Contact Lecture Hours: 90

Course outcomes

- To analyse and apply various instrumental methods and analytical procedures to molecular systems.
- To understand the importance of application of analytical techniques in environmental monitoring
- To gain expertise on various sampling techniques
- To define and describe basic principles of capillary electrophoresis and capillary electro chromatography and demonstrate their applications
- To have an idea about renewable and non renewable aquatic resources.

Module I: Instrumental Methods (36 Hours)

1.1 Electrical and nonelectrical data domains-transducers and sensors, detectors, examples for piezoelectric, pyroelectric, photoelectric, pneumatic and thermal transducers. Criteria for selecting instrumental methods-precision, sensitivity, selectivity, and detection limits.

1.2 Signals and noise: sources of noise, S/N ratio, methods of enhancing S/N ratiohardware and software methods.

1.3 Electronics: transistors, FET, MOSFET, ICs, OPAMs. Application of OPAM in amplification and measurement of transducer signals.

1.4 UV-Vis spectroscopic instrumentation: types of optical instruments, components of optical instruments - sources, monochromators, detectors. Sample preparations, Instrumental noises, applications in qualitative and quantitative analysis.

1.5 Molecular fluorescence and fluorometers: photoluminiscence and concentrationelectron transition in photoluminescence, factors affecting fluorescence, instrumentation details. Fluorometric standards and reagents. Introduction to photoacoustic spectroscopy.

1.6 IR spectrometry: instrumentation designs-various types of sources, monochromators, sample cell considerations, different methods of sample preparations, detectors of IRNDIR instruments. FTIR instruments, Mid IR absorption spectrometry. Determination of path length. Application in qualitative and quantitative analysis.

1.7 Raman Spectrometric Instrumentation: sources, sample illumination systems. Application of Raman Spectroscopy in inorganic, organic, biological and quantitative analysis.

1.8 NMR Spectrometry-magnets, shim coils, sample spinning, sample probes (^{1}H, ^{13}C, ^{32}P). Principle of MRI.

Module II: Sampling (18 Hours)

2.1 The basis and procedure of sampling, sampling statistics, sampling and the physical state, crushing and grinding, the gross sampling, size of the gross sample, sampling liquids, gas and solids (metals and alloys), preparation of a laboratory sample, moisture in samples-essential and non essential water, absorbed and occluded water, determination of water (direct and indirect methods).

2.2 Decomposition and dissolution, source of error, reagents for decomposition and dissolution like HCl, H_2SO_4, HNO_3, $HClO_4$, HF, microwave decompositions, combustion methods, use of fluxes like Na_2CO_3, Na_2O_2, KNO_3, NaOH, $K_2S_2O_7$, B_2O_3 and lithium metaborate. Elimination of interference from samples-separation by precipitation, electrolytic precipitation, extraction and ion exchange. Distribution ratio and completeness of multiple extractions.Types of extraction procedures.

Module III: Applied Analysis (9 Hours)

3.1 Analytical procedures involved in environmental monitoring. Water quality-BOD, COD, DO, nitrite, nitrate, iron, fluoride.

3.2 Soil-moisture, salinity, colloids, cation and anion exchange capacity.

3.3 Air pollution monitoring sampling, collection of air pollutants-SO_2, NO_2, NH_3, O_3 and SPM.

3.4 Analysis of metals, alloys and minerals. Analysis of brass and steel, Analysis of limestone, Corrosion analysis.

Module IV: Capillary Electrophoresis and Capillary Electro Chromatography (9 Hours)

4.1 Capillary electrophoresis-migration rates and plate heights, instrumentation, sample introduction, detection (indirect)-fluorescence, absorbance, electrochemical, mass spectrometric, applications. Capillary gel electrophoresis, Capillary isotachophoresis, Isoelectric focusing.

4.2 Capillary electro chromatography-packed columns. Micellar electro kinetic chromatography.

Module V: Process Instrumentation (9 Hours)

5.1 Automatic and automated systems, flow injection systems, special requirements of process instruments, sampling problems, typical examples of C, H and N analysers.

Module VI: Aquatic Resources (9 Hours)

6.1 Aquatic resources: renewable and non renewable resources, estimation, primary productivity and factors affecting it, regional variations.

6.2 Desalination: principles and applications of desalination-distillation, solar evaporation, freezing, electrodialysis, reverse osmosis, ion exchange and hydrate formation methods. Relative advantages and limitations. Scale formation and its prevention in distillation process.

6.3 Non-renewable resources: inorganic chemicals from the sea-extraction and recovery of chemicals, salt from solar evaporation.

References

1. J.M. Mermet, M. Otto, R. Kellner, Analytical Chemistry, Wiley-VCH, 2004.
2. D.A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, Fundamentals of Analytical Chemistry, 8th Edn., Saunders College Pub., 2007.
3. R.D. Brownn, Introduction to Instrumental Analysis, McGraw-Hill, 1958.
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6. J.H. Kennedy, Analytical Chemistry: Principles, Saunders College Pub., 1990.
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8. E.D. Howe, Fundamentals of Water Desalination, Marcel Dekker, 1974.
9. H.G. Heitmann, Saline Water Processing, VCH


FOR TRUTH AND SERVICE

MEDICINAL CHEMISTRY (PCH4CRT0622)

Credit : 4 Contact Lecture Hours: 90

Course outcomes

- To Classify the drugs with examples and structures
- To study themode of action of drugs in biological systems.
- To describe the structure activity relation of some important class of drugs
- To explain the drugs used for various infectious diseases caused by pathogens
- To describe Therapeutic uses of drugs and Precise side effect of 'Drug Substances'

Module I: Drugs Acting on ANS (18 Hours)

1.1 Adrenergic stimulants: Phenyl ethanolamine derivatives-adrenaline, isoprenaline, salbutamol, ephedrine, and phenylephrine. Imidazole derivatives-naphazoline, xylometazoline and oxymetazoline.

1.2 Adrenergic blockers: α and β adrenoreceptor antagonists-ergot alkaloids, phenoxybenzamine, phentolamine, tolazoline, DCI, propranolol, atenolol, labetololNeurone blockers–Bretilium and Xylocholine.

1.3 Cholinergic stimulants: nicotinic and muscarinic receptors, acetyl choline andanalogues, pilocarpine, bethanechol and carbachol.

1.4 Cholinergic blockers: tertiary and quaternary antimuscarinics, antispasmodic drugsdicyclomine, glycopyrrolate, antiulcer drugs-pirenzepine, cycloplegic drugstropicamide, homatropine

1.5 Anticholinesterases: Competitive inhibitors-physostigmine and neostigmine.

1.6 Non-competitive inhibitors: organophosphorus compounds, Nerve gases,Cholinesterase regenerators-2 PAM.

1.7 Ganglion blocking agents: mecamylamine and trimethophan

1.8 Curareform drugs: curare alkaloids, erythrina alkaloids and gallamine.

1.9 Synthesis of the following drugs: salbutamol, naphazoline, tolazoline, propranolol,bretilium, carbachol, mecamylamine and gallamine.

Module II: Drugs Acting on CVS (9 Hours)

2.1 Cardiotonic drugs: cardiac glycosides-their chemistry and stereochemistry, Digoxin and digitoxin.

2.2 Antiarrhythmic drugs: quinidine, disopyramide, lidocaine, phenytoin andprocainamide, β-blockers-propranolol. Calcium channel blockers-verapamil and Neurone blockers-bretilium.

2.3 Antihypertensive Drugs: peripheral antiadrenergics-prazosin and terazosin. Centrallyacting drugs-reserpine, clonidine and methyl dopa. β-blockers- propranolol, atenololand labetalol. Calcium channel blockers-nifedipine and amlodipine. ACE inhibitors captopri.Angiotensin receptor blockers-losartan.Diuretics-thiazide diuretics.

2.4 Antianginal drugs: vasodilators-nitrites and nitrates, β-blockers-propranolol. Calcium channel blockers-verapamil and nifedipine. Miscellaneous-dipyridamol and aspirin.

2.5 Anticoagulants: heparin, coumarin derivatives and indanedione derivatives.

2.6 Antilipidemic agents: atherosclerosis (mention only), Statins-lovastatin, simvastatin, fluvastatin, Fibrates-clofibrate, Miscellaneous-bile acid sequestrants andcholestyramine resin.

2.7 Synthesis of the following drugs: procainamide, disopyramide, amlodipine, verapamil, captopril and fluvastatin.

Module III: Chemotherapy (27 Hours)

3.1 Antibiotics: β-lactam antibiotics-penicillins and cephalosporins, natural, biosyntheticand semisynthetic penicillins, tetracyclines and chloramphenicol, a brief study ofmacrolide antibiotics, aminoglycoside antibiotics, polyene antibiotics, fluoro quinolones.

3.2 Sulphonamides: sulphanilamide, N-substituted sulphanilamide derivatives, mechanism of action, sulphones-dapsone, dihydrofolate reductase inhibitors trimethoprim and cotrimoxazole.

3.3 Antitubercular agents: first line drugs-isoniazid, rifampicin, pyrazinamide, ethambutol, and streptomycin. Second line drugs-ethionamide, para amino salicylic acid and fluoro quinolones.

3.4 Antifungal agents: Antibiotics-amphotericin B, griseofulvin and nystatin. Azolederivatives-ketoconozole, terconozole, fluconozole and clotrimazole. Pyrimidine derivatives - 5 Flucytosine.

3.5 Antiviral drugs: amantidine, interferon and ribavirin. Anti HIV agents- zidovudine, andabacavir. Anti-herpes simplex agents-brivudine, vidarabin and acyclovir. Antiinflueza agents-oseltamivir(tamiflu).

3.6 Antiprotozoal agents: Amoebicides-metranidazole and tinidazole. Antimalarial schloroquine, primaquine, mefloquine, quinacrine and proguanil. Anthelmintics piperazines and benzimidazoles. Miscellaneous-eflornithine and pentamidine. Synthesis of the following drugs: ampicillin, cephalexin, chloramphenicol, sulphamethoxazole, dapsone, trimethoprim, ethambutol, griseofulvin, clotrimazole, acyclovir, metranidazole, primaquine, mebendazole.

Module IV: Antineoplastic Drugs (9 Hours)

4.1 Neoplasm-cause therapeutic approaches. Alkylating agents-nitrogen mustards, nitrosourea, aziridines and aryl sulphonates.Antimetabolites-folic acid.Antagonistspurine and pyrimidine antagonists. Antibiotics-anthracyclines, actinomycin D,bleomycin. Plant products-vinca alkaloids, taxol derivatives. Hormones and their antagonists-tamoxifen. Miscellaneos-procarbazine, cisplatin.

4.2 Synthesis of the following drugs: chlorambucil, carmustin, thiotepa, methotrexate, 5-fluoro uracil, procarbazine.

Module V: Psychopharmocological Agents (9 Hours)

5.1 Tranquilisers: rauwolfia alkaloids, meprobamate, oxazepim, benzodiazepines, chlordiazepoxide, phenothiazene derivatives.

5.2 Antidepressants: MAO inhibitors-Isocarboxazide, tranylcypromine and phenelzine.

Tricyclic compounds - imipramine, trimipramine, amitriptynine, doxepine, amoxapine. Miscellaneous compounds-fluoxetine and trazodone.

5.3 Antipsychotics: phenothiazine and thiothixene derivatives, butyrophenones haloperidol, droperidon, rauwolfia alkaloids.

5.4 Hallucinogens: triptamine derivatives - DMT, psilocybin, phenylalkylamines mescaline, lysergic acid derivatives - LSD.

5.5 Synthesis of the following drugs: chlordiazepoxide, meprobamate, imipraminechlorpromazine, tranylcypromine and haloperidol.

Module VI: Miscellaneous Class of Compounds (18 Hours)

6.1 Diuretics: common diuretics and their mechanism of action - mercurial andnonmercurial diuretics, carbonic anhydrase inhibitors - acetazolamide and methazolamide, thiazide derivatives-hydrochlorothiazide, Loop diuretics- furosemide and ethacrynic acid, potassium sparing diuretics-amiloride, spironolactone.

6.2 Antihistaminic drugs: histamine and its biological role, H1 antagonists-aminoalkylethers, diphenhydramine and doxylamine, ethylenediamine derivatives-pyrilamine, phenothiazines-promethazine, trimeprazine, piperazine derivatives-cyclizines, miscellaneous compounds-cetrizine and cyproheptadine.

6.3 Hypogycemic agents: type 1 and type 2 diabetes, insulin, suphonyl ureastolbutamide, acetohexamide and glibenclamide, biguanides-metformin, thiazolidinediones-rosiglitazone.

6.4 Local anaesthetics: clinical application of local anaesthesia, coca and cocaine, hexylcaine, paraaminobenzoic acid derivative-benzocaine, procaine, tetracaine, chloroprocaine, anilides, lidocaine, etiodacaine and prilocaine.

6.5 Antitussives: centrally acting antitussives-opium alkaloids and synthetic substitutes codaine, noscapine, pholcodine, ethylmorphine, dextromethorphan, Non narcoticantitussives-diphenhydramine, expectorants-terpin hydrate, guaicol and bromhexine.

6.6 Gastrointestinal drugs: purgatives-irritant, osmotic, bulk and lubricant purgatives, Antacids-systemic and non-systemic antacids, H2 antagonists-cimetidine andranitidine, proton pump inhibitors-omeprazole and pantoprazole, digestants, carminatives and antidiarrheals.

6.7 Synthesis of the following drugs: acetazolamide, chlorthiazide furosemide, ethacrynicacid, amiloride, diphenhydramine, pyrilamine, promethazine, omeprazole, tolbutamide, phenformin, benzocaine, procaine lidocaine, dextromethorphan.

References

1. G.L. Patrick, Medicinal Chemistry, BIOS, 2001.

2. T. Nogrady, D.F. Weaver, Medicinal Chemistry, Oxford University Press, 2005.

3. W.O. Foye, T.L. Lemke, D.A. Williams, Principles of Medicinal Chemistry, 4th Edn.Williams & Wilkins, 1995.

4. J.P. Remington, Remington's Pharmaceutical Sciences, Vol.13, 19th Edn. Mack,1990.

5. D. Sriram, P.Yogeswari, Medicinal Chemistry, Pearson Education India, 2010.

6. K.D. Tripathi, Essentials of medical Pharmacology, 6th Edn. Jaypee, 2008

7. L.S. Goodman, A. Gillman, The Pharmacological Basis of Therapeutics, 10th Edn.McGraw Hill, 2001.

8. S.S. Kadam, Principles of Medicinal Chemistry, Vol.I& II, Pragati Books, 2008.

9. A. Kar, Medicinal Chemistry, New Age International, 2007.

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Practicals - Semesters III & IV

INORGANIC CHEMISTRY PRACTICALS - 2 (PCH3CRP0122/PCH4CRP0122)

108 Hours 3 Credits

Course Outcomes

After successful completion of the course, the students should be able to

- Acquire laboratory skill in the estimation of simple metal ions by volumetric titrations
- Attain laboratory skill in the analysis of alloys; brass, bronze and solder
- Acquire laboratory skills in the paper chromatographic separation of cations
- Perform preparation of complexes of Co(III) and Ni(II) and study the *cis-trans* isomerisation of the former by UV spectroscopy
- Perform estimation of the equilibrium constant of substitution of Fe(III) using calorimeter or UV spectrophotometer

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, illmenite.

Part III

Paper chromatographic separation of a mixture of 3 cations.

a) Separation of Ag(I), Pb(II) and Hg(II)ions

b) Separation of Ni(III), Co(II) and Zn(II)ions

c) Separation of Ni(III), Co(II) and Cu(II)ions

d) Separation of Ba(II), Sr(II) and Ca(II)ions

Part IV

Preparation of cis and trans-Dichlorobis(ethylenediamine)cobalt(III) chloride and kinetic study of cis to trans isomerisation using a UV-Vis spectrophotometer.

Synthesise the following complexes of Ni(II) (a d^8 system) and prepare 0.05 M solutions of the complexes in the solvents specified.

Complex	Solvent and Blank.	Concentration
1. $[Ni(bipy)_3]SO_4.6H_2O$	Water	0.05M
2. $[Ni(en)_3]Cl_2.2H2O$	20% en	0.05M
3. $[Ni(NH_3)_6]Cl_2$	Aqueous NH_3	0.05M
4. $[Ni(H_2O)_6]SO_4$	Water	0.05M
5. $[Ni(DMSO)_6](ClO_4)_2$	DMSO	0.05M
6. $K_4[Ni(NCS)_6]4H_2O$	10M KSCN in water	0.05M

Record the electronic spectrum of each solution in the region 200 – 1100 nm. Calculate Δ values for all six complexes. Arrange the ligands in the spectrochemical series i.e. in the order of increasing Δ.

Estimation of equilibrium constant of the reaction, $Fe^{3+} + SCN^- \leftrightarrow FeSCN^{2+}$ with the help of a colorimeter or UV-VIS spectrophotometer.

References

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., Mc Millian,1968.
3. G. Pass, H. Sutcliffe, Practical Inorganic Chemistry, Chapman & Hall,1974.
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7. Journal of Chem. Ed. , 1962, 39, 634. 8. J.C.S. 1953,2696.
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9. Sutton, J. Chem. Educ. 1960, 37,498.
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ORGANIC CHEMISTRY PRACTICALS - 2 (PCH3CRP0222/PCH4CRP0222)

108 Hours 3 Credits

Course Outcomes

After successful completion of the course, the students should be able to

- Acquire laboratory skill in multi step organic synthesis
- Attain laboratory skill green organic synthesis
- Perform microwave assisted organic synthesis
- Perform estimation of organic compounds using UV spectrophotometer
- Characterize the synthesized compounds by IR, UV-Vis and NMR spectroscopy

Part I

Preparation Involving Two step Synthetic Sequences by Chemical Methods

Chem Draw/Chem Sketch, Reaction stoichiometry, execution of the reaction, monitoring by TLC, work-up, purification, yield calculation and characterization

Meta-nitrobenzoic acid from methylbenzoate

Paranitroaniline from acetanilide

1,3,5 -tribromoaniline from acetanilide

Parabromoaniline from acetanilide

Benzanilide from benzophenone

Schiff's base from aniline

Paracetamol from phenol

Phenol from aniline

Methyl red from anthranilicacid

Para nitrobenzoic acid from toluene

Part II

Spectrophotometric (UV-Vis) estimations of organic compounds (eg: Nitro compounds, azo compounds etc.)

Part III

Preparation Involving Multistep Synthetic Sequences by the Green Alternatives of Chemical Methods

1,1-bis -2-naphthol from2-naphthol

Benzopinacol frombenzophenone

Benzopinacolone fromBenzopinacol

o-Methyl acetanilide fromo-toludine

Acetanilide fromaniline

Part IV

Microwave assisted Organic Synthesis

Benzoic acid from ethylbenzoate

Benzoic acid from benzyl alcohol

Ethyl-3-nitrobenzoate from 3-nitrobenzoicacid

2-hydroxychalcone fromsalicylaldehyde

Anthracene-maleic anhydrideadduct

Part V

Prediction of FTIR, UV-Visible, ^{1}H and ^{13}C NMR spectra of the substrates and products at each stage of the products synthesized by the above methods.

References

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 and B.C Saunders, Practical Organic Chemistry, 4th Edn., Pearson

Education India,2009.

4. J.R. Adams, J.R. Johnson, J.F. Wilcox, Laboratory Experiments in Organic Chemistry, Macmillan,1979.
5. V.K. Ahluwalia, Green Chemistry: Environmentally Benign Reactions, Ane Books, 2009.
6. Monograph on Green Chemistry Laboratory Experiments, Green ChemistryTask Force Committee, DST, 2009.

PHYSICAL CHEMISTRY PRACTICAL– 2 (PCH3CRP0322/PCH4CRP0322)

144 Hours 3 Credits

Course Outcomes

After successful completion of the course, the students should be able to

- Acquire laboratory skill in the determination of rate constant of hydrolysis reactions
- Attain laboratory skill in kinetics/concentration estimations of sugars and acids by polarimetry
- Perform experiments involving refractometry like determination of concentration of KCl-water/ glycerol-water.
- Perform experiments for the determination of viscosity/concentration using viscosity.
- Carryout conductometric and potentiometric titration experiments involving acids and bases.

1. Chemical Kinetics

Determination of the rate constant of the hydrolysis of ester by sodium hydroxide

Determination of the rate constant of the hydrolysis of ester by acid

Kinetics of reaction between $K_2S_2O_8$ and KI.

2. Polarimetry

Kinetics of the inversion of sucrose in presence of HCl.

Determination of the concentration of a sugar solution

Determination of the concentration of HCl

Determination of the relative strength of acids

3. Refractometry

Identification of pure organic liquids and oils

Determination of molar refractions of pure liquids

Determination of concentration of solutions (KCl-Water, Glycerol-Water)

Determination of molar refraction of solids

Study of complex formation between potassium iodide and mercuric iodide system

4. **Viscosity**

Determination of viscosity of pure liquids

Verification of Kendall's equation-full experiment

Determination of composition of binary liquid mixture (toluene-nitro benzene)

Determination of molecular weight of a polymer (polystyrene in toluene)

5. **Conductance Measurements**

Titration of a dibasic acid against strong base

Titration of a mixture of acids against a strong base

Titration of weak acid vs strong base

Verification of Onsagar equation

Determination of dissociation constant of a weak acid

6. **Potentiometry**

Titration of strong acid vs strong base

Titration of weak acid vs strong base

Titration of a mixture of acids against a strong base

Application of Henderson equation

Determination of single electrode potential (Cu and Zn)

References

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

4. Dr. J. N. Gurtu & Amit Gurtu ADVANCED PHYSICAL CHEMISTRY EXPERIMENTS

GIST OF CHANGES

Semester	Paper	Unit	Changes	
			Existing	**Modified**
I	STRUCTURAL AND MOLECULAR ORGANIC CHEMISTRY COURSE NAME CHANGED TO ORGANIC CHEMISTRY-1	Unit 1	Basic Concepts in Organic Chemistry (18 Hrs)	No change
		Unit 2	Physical Organic Chemistry (9 Hrs)	No change
		Unit 3	Organic Photochemistry (9 Hrs)	No change
		Unit 4	Stereochemistry of Organic Compounds (18 Hrs)	Change Akampptisomerism to Atropisomerism
		Unit 5	Conformational Analysis (18 Hrs)	Removed conformational analysis of sucrose and lactose

Semester	**Paper**	**Unit**	**Changes**	
			Existing	**Modified**
II	ORGANIC REACTION MECHANISMS COURSE NAME CHANGED TO ORGANIC CHEMISTRY-II	Unit 1	Review of Organic Reaction Mechanisms (9 Hrs)	No change
		Unit 2	Chemistry of Carbanions (9 Hrs)	No change
		Unit 3	Chemistry of Carbocations (9 Hrs)	No change
		Unit 4	Carbenes, Carbenoids, Nitrenes and Arynes (9 Hrs)	No change
		Unit 5	Radical Reactions (9 Hrs)	No change
		Unit 6	Chemistry of Carbonyl Compounds (9 Hrs)	No change
		Unit 7	Concerted Reactions	Include electro cyclic reactions in

			(18 hrs)	detail
Semester	**Paper**	**Unit**	**Changes**	
			Existing	**Modified**
III	ORGANIC SYNTHESES COURSE NAME CHANGED TO ORGANIC CHEMISTRY-III	Unit 1	Organic Synthesis via Oxidation and Reduction (18 Hrs)	No change
		Unit 2	Modern Synthetic Methods (18Hrs)	No change
		Unit 3	Synthetic Reagents (9 Hrs)	No change
		Unit 4	Construction of Carbocyclic and Heterocyclic Ring Systems (9 Hrs)	No change
		Unit 5	Protecting Group Chemistry (9 Hrs)	No change
		Unit 6	Retrosynthetic Analysis (9 hrs)	Unit moved to Sem 4 Research Methodology

				(shifted from Unit 8, Semester 4) *Journal Club – as seminar*
Semester	**Paper**	**Unit**	**Changes**	
			Existing	**Modified**
IV	ADVANCED ORGANIC CHEMISTRY	Unit 1	Molecular Recognition and Supramolecular Chemistry (18 Hrs) Changed to Supramolecular Chemistry and advanced polymer chemistry	Module name changed to Supramolecular Chemistry and advanced polymer chemistry Removed topics - lariat ethers, podands and spherands from cation binding hosts Only elementary structural features of tweezers, molecular clefts, macrocyclic polyamines and siderphores.

				Included topics from module 7 (advances in polymer chemistry)
		Unit 2	Green Alternatives to Organic Synthesis (9 Hrs)	No change
		Unit 3	Biosynthesis and Biomimetic Synthesis (9 Hrs)	No change
		Unit 4	Stereoselective Transformations (9 Hrs)	No change
		Unit 5	Chemistry of Natural Products and Biomolecules (18 Hrs)	Removed synthesis of cyanin and testosterone Topic on Carbohydrate has to be added as 5.2 Proteins and nucleic acids are

				added as 5.3
		Unit 6	Medicinal Chemistry and Drug Designing (9 Hrs)	No change
		Unit 7	Advances in Polymer Chemistry (9 Hrs) Changed as Retrosynthetic Analysis	Removed Advances in Polymer Chemistry to unit 1 and introduced retrosynthesis from semester 3 with minor changes Removed amine and alkene synthesis Instead of 'luciferin' organic molecules Remove special mention of Ireland-Claisen rearrangement
		Unit 8	Total syntheses (9 Hrs)	Introduced new unit which

				includes synthesis of 7 biologically important / natural products.
III & IV	PCH3CRP0219/PCH4CRP0219 ORGANIC CHEMISTRY PRACTICAL -2	Part III	*OR*	Chem Draw/Chem Sketch, Reaction stoichiometry, execution of the reaction, monitoring by TLC, work-up, purification, yield calculation and characterization

Semester	**Paper**	**Unit**	**Changes**	
			Existing	**Modified**
I	THERMODYNAMICS, KINETIC THEORY AND STATISTICAL THERMODYNAMICS (54 Hrs) (There is no change for total credits and workload)	Unit 1	Classical Thermodynamics (18 Hrs)	No change
		Unit 2	Kinetic Theory of Gases (9 Hrs)	Replaced "*Collision frequency in a single gas and mixture of gases, mean free path, frequency of collision*" by

				Collision frequency, mean free path
		Unit 3	Statistical Thermodynamics (27 Hrs)	No change
III	PCH3CRT0319 CHEMICAL KINETICS, SURFACE CHEMISTRY AND CRYSTALLOGRAPHY Credit: 4 Contact Lecture Hours: 72	Unit 1	Chemical Kinetics (27 Hrs)	No change
		Unit 2	Surface Chemistry (27 Hrs)	No change
		Unit 3	Crystallography (18 Hrs)	No change
IV	PCH4CRT0319 ADVANCED PHYSICAL CHEMISTRY Credit: 4 Contact Lecture Hours: 90	Unit 1	Photochemistry (18 Hrs)	No change
		Unit 2	Fluorescence Spectroscopy (9 Hrs)	No change
		Unit 3	Diffraction Methods and Atomic Spectroscopic Techniques (9 Hrs)	No change

		Unit 4	Electrochemistry and Electromotive Force (27 Hrs)	Removed- *Corrosion and methods of prevention, Pourbaix diagram and Evans diagrams. (2 hours)* Added- *Solubility product principle, solubility in the presence of common ion, activity coefficient and solubility measurement, determination of activity coefficient from equilibrium constant measurement* *(2 hours)*
		Unit 5	Electroanalytical Techniques (18 Hrs)	No change

		Unit 6	Advanced Thermodynamics (9 Hrs)	No change

Journal Club

Choose a recent research article of their choice published in any reputed international journal and go through it thoroughly.

a) Abstract in their own words.

b) Why is the article important? / What is the pre-existing knowledge in the topic?

c) What is the novelty of the work done? / What are the new findings?

d) What sort of data supports the findings?

e) Conclusion in their own words.

f) How does the article boost further research on the topic?

Apart from these, the students should do a PowerPoint presentation on the paper in the presence of other students and concerned teachers of the department. Students and teachers may ask questions like a Master thesis defence. It may be scheduled in such a way that one presentation of duration one hour takes place per week.