GNA UNIVERSITY
SRI HARGOBINDGARH, PHAGWARA – HOSHIARPUR ROAD,
PHAGWARA 144401, PUNJAB

ORDINANCE

FOR

MASTER OF SCIENCE – CHEMISTRY

GNA UNIVERSITY
Inspiring Innovation.....

(THIS ORDINANCE HAS BEEN APPROVED IN THE MEETING OF BOARD OF STUDIES HELD ON DATED 31st May, 2022)

APPLICABLE W.E.F. ACADEMIC SESSION 2022-2023

SRI HARGOBINDGARH, PHAGWARA – HOSHIARPUR ROAD,PHAGWARA 144401, PUNJAB

ORDINANCE FOR M.SC. CHEMISTRY

SHORT TITLE AND COMMENCEMENT

I. This Ordinance shall be called the Ordinance for the M.Sc. Chemistry Program of GNA University, Phagwara.

II. This Ordinance shall come into force with effect from academic session 2022 - 23

1. Name of Program: M.Sc. Chemistry

2. Name of Faculty: Faculty of Natural Sciences.

3. Vision of the department: To Produce highly qualified academician and researcher in the field of chemistry accepting globally for catering the need of the industry as well as society.

4. Mission of the department:

M1: To prepare students with practical &technical aspects of chemistry, which they are ready to take the new real-world challenges.

M2: Establish an industry-academia relationship to enhance the technical skills of students to work prominently in industrial environments.

M3: Provide exposure to students of state-of-the-art tools and technology in the field of chemistry

M4: Each Faculty member motivates students to become problem-solving individuals, researcher, a good academician in the field of chemistry.

5. Program Educational Outcomes (PEO):

PEO1: To prepare students who will be successful professionals in industry, government, academia, research, entrepreneurial pursuit, and consulting firms.

PEO2: To prepare students who will contribute to society as broadly educated, expressive, ethical, and responsible citizens with proven expertise.

PEO3: To prepare students who will achieve peer-recognition; as an individual or in a team; through demonstration of good analytical, design and implementation skills.

PEO4: To prepare students who will thrive to pursue life-long learning to fulfill their goals

6. Program Outcomes (PO):

Po1: Computational Knowledge: Apply knowledge of chemicals, salts, its practical approach using mathematics to the abstraction and conceptualization of chemical structures from defined problems and requirements.

PO2: Problem Analysis: Identify, formulate, research literature, and solve complex computing problems reaching substantiated conclusions using fundamental principles of chemistry.

PO3: Design/Development of Solutions: Design and evaluate solutions for complex problems, and design and evaluate systems, theoretical & practical's that meet specified needs with appropriate consideration for public health and safety, cultural, societal, and environmental considerations.

Po4: Conduct investigations of complex Computing problems: Use research-based knowledge and research methods including design of experiments, analysis and interpretation of data,and synthesis of the information to provide valid conclusions.

PO5: Modern Tool Usage: Create, select, adapt, and apply appropriate techniques, resources, and modern computing tools to complex computing activities, with an understanding of the limitations.

PO6: Professional Ethics: Understand and commit to professional ethics and cyber regulations, responsibilities, and norms of professional computing practices.

PO7: Life-long Learning: Recognize the need, and have the ability, to engage in independent learning for continual development as a researcher or professional.

PO8: Communication Efficacy: Communicate effectively with the community, and with society at large, about complex computing activities by being able to comprehend and write effective reports, design documentation, make effective presentations, and give and understand clear instructions.

PO9: Societal and Environmental Concern: Understand and assess societal, environmental, health, safety, legal, and cultural issues within local and global contexts, and the consequential responsibilities relevant to professional practices.

PO11: Individual and Teamwork: Function effectively as an individual and as a member or leader in diverse teams and in multidisciplinary environments.

PO12: Innovation and Entrepreneurship: Identify a timely opportunity and using innovation to pursue that opportunity to create value and wealth for the betterment of the individual and society at large

7. Program Specific Outcomes (PSO):

PSO1: Understand the concepts and applications in the field of chemical sciences, drugs, pharmacy, starch industry, paper industry, dye industry, etc.

PSO2: Apply the learning from the courses and develop applications for real world problems.

PSO3: Understand the technological developments in the usage of modern design and development tools to analyze and design for a variety of applications.

PSO4: Communicate in both oral and written forms, demonstrating the practice of professional ethics and the concerns for social welfare.

8. General Regulations for Faculty of Natural Sciences:

8.1 The University may introduce programs under Faculty of Natural Sciences which are specified under the UGC Act 1956. The Governing Body may approve the introduction, suspending or phasing out a program on the recommendation of the Academic Council either on its own or on the initiative of faculty.

8.2 The admissions to a Faculty of Natural Sciences programs shall be generally governed by the rules of the UGC or any other competent authority of the MHRD or as approved by Governing Body of University and shall be as notified in the admission notification of the respective academic year.

8.3 The minimum entry qualification for admission to the students of Faculty of Natural Sciences shall be such as may be laid down in the regulations or specified by the Governing Body like Minimum qualification for admission to the first year program of Faculty of Natural Sciences shall be the Senior Secondary School Certificate (10+2) examination. While deciding the admission procedure, the University may lay down compulsory subjects in qualifying examination for admission for various programs in the admission policy.

8.4 A student shall be required to earn a minimum number of credits through various academic components of a curriculum, as provided for in the regulations.

8.5 A student shall be required to complete all the requirements for the award of the degree within such period as may be specified in the regulations.

8.6 A student may be granted such scholarship as may be specified in accordance with the

8.7 A student admitted to the programs shall be governed by the rules, regulations and procedures framed and implemented by the University from time to time.

8.8 The students shall abide by the regulations mentioned in student handbook issued by the University. These standing regulations shall deal with the discipline of the students in the Hostels, Faculty, and University premises or outside. The standing orders may also deal with such other matters as are considered necessary for the general conduct of the students' co-curricular and extra-curricular activities.

8.9 In exceptional circumstances the chairman of Academic Council may, on behalf of the Council, approve amendments, modifications, Insertions or deletions of an Ordinance(s) which in his/her opinion is necessary or expedient for the smooth running of the program provided all such changes are reported approved to the Council in its next meeting.

9. General Regulations for the M.Sc. Chemistry:

9.1 Short Title and Commencement: These regulations shall be called regulations for the PG programs in Faculty of Natural Sciences of the University and shall come into force on such a date as the Academic Council may approve.

9.2 Duration: The duration of the PG programs leading to degrees of M.Sc. Chemistry shall be minimum two years and each year will comprise of two semesters. However, the duration may be extended up-to five years from the registered batch. The maximum duration of the programs excludes the period of withdrawal, due to medical reasons. However, it shall include the period of rustication or any other reason of discipline /academics e.g. detention, willful absence by the student, not getting promotion to the next class due to poor academic performance etc. Under detention, the student shall attend the University for an additional semester or more time, as equated to period of absence/suspension.

9.3 Starting or Phasing out of Program: A program may be phased out on recommendations of the Academic Council and approval of the Governing Body, on account of continuous low registration in the program or any other justifiable reason like becoming obsolete etc. Similarly, the Academic Council may approve starting of a new program or modifying the existing one on the recommendations of the Academic Council.

9.4 Admissions: The centralized admission cell shall make selection for admission to the program. Admission to this program shall be made as per procedure to be approved by the Academic Council, and further by Board of Management and Governing Body and may be reviewed periodically as required. Eligibility criteria for the program, meriting and selection policy, fee structure, refund policy, total number of seats etc. shall be defined in the admission policy.

9.5 Eligibility for Admission: B.Sc. Non medical/ B.Sc. Medical/ B.Sc. (Honours) Chemistry. with 50% marks in aggregate (45 % for SC/ST/OBC).

9.6 Semester System: The M.Sc. Chemistry academic programs in the University shall be based on Semester System, namely, Even (Jan to June) and Odd (July to Dec) Semesters, in an academic year. The courses whether offered in regular semester shall be evaluated as per the policy and procedure laid down.

9.7 Semester Duration: Total duration of the Program shall be of two years and each year will comprise of two semesters. In addition, each semester shall normally have teaching for the 90 working days.

10. Curriculum: The two years curriculum has been divided into four semesters and shall include lectures, tutorials, practical, and projects along with the industrial visits and educational tours etc. The curriculum will also include other curricular, co-curricular and extra-curricular activities as may be prescribed by the University from time to time.

11. Choice Based Credit System:

The University has adapted Choice Based Credit System (CBCS) which provides an opportunity for the students to choose courses from the prescribed courses comprising core, elective/minor courses. The choice based credit system provides a “flexible” approach in which the students can take courses of their choice, learn at their own pace, undergo additional courses and acquire more than the required credits, and adopt an interdisciplinary approach to learning. Following are the types of courses and structure for the program:

11.1 Core Course: A course, which should compulsorily be studied by a candidate as a core requirement is termed as a core course.

11.2 Core Laboratory: A laboratory which should be compulsorily be studied by a candidate as a core requirement is termed as core Laboratory.

11.3 Elective Course: Generally a course which can be chosen from a pool of courses and which may be very specific or specialized or advanced or supportive to the discipline/subject of study or which provides an extended scope or which enables an exposure to some other discipline/subject/domain or nurtures the candidate's proficiency/skill is called an Elective Course.

I. Elective Course: Elective courses may be offered by the main discipline/subject of study is referred to as Elective courses. The University/Institute may also offer discipline related Elective courses of interdisciplinary nature (to be offered by main discipline/subject of study).

ii. Project work/Dissertation is considered as a special course involving application of knowledge in solving / analysing /exploring a real life situation / difficult problem. A Project/Dissertation work would be of 5 credits. A Project/Dissertation work may be given in lieu of a discipline specific elective paper.

12. Medium of Instructions:

12.1 The medium of instruction for M.Sc. Chemistry will be English.

12.2 Question Papers of all examinations will be set and answered in English.

12.3 Practical work/Project Work / Project Report / Dissertation / Field Work Report / Training Report etc., if any, should be presented in English.

13. Mode: The program is offered on 'Full Time' mode of study only.

14. Attendance Requirement to be Eligible to Appear in End Semester Examination:

14.1 Every student is required to attend at least 75% of the lectures delivered squaring tutorials, practical and other prescribed curricular and co-curricular activities.

14.2 Dean of Faculty may give a further relaxation of attendance up to 10% to a student provided that he/she has been absent with prior permission of the Dean of the Faculty for the reasons acceptable to him/her.

14.3 Further, relaxation up to 5% may be given by the Vice Chancellor to make a student eligible under special circumstances only.

14.4 No student will be allowed to appear in the end semester examination if he/she does not satisfy the attendance requirements. Further, the attendance shall be counted from the date of admission in the University or commencement of academic session whichever is later.

14.5 Attendance of N.C.C/N.S.S. Camps or Inter-Collegiate or Inter-University or Inter-State or International matches or debates or Educational Excursion or such other Inter-University activities as approved by the authorities involving journeys outside the city in which the college is situated will not be counted as an absence. However, such absence shall not exceed four weeks per semester of the total period of instructions. Such type of facility should not be availed twice during the study.

15. Credit: Each course, except a few special audit courses, has a certain number of credits assigned to it depending upon its lecture, tutorial and/or laboratory contact hours in a week.

A letter grade, corresponding to a specified number of grade points, is awarded in each course for which a student is registered. On obtaining a passing grade, the student accumulates the course credits as earned credits. A student's performance is measured by the number of credits that he/she has earned and by the weighted grade point average. A minimum number of credits should be acquired to qualify for the programs.

Earned Credits (EC): The credits assigned to a course in which a student has obtained 'D' (a minimum passing grade) or a higher grade will be counted as credits earned by him/her. Any course in which a student has obtained F, or W or "I" grade will not be counted towards his/her earned credits.

A unit by which the course is measured. It determines the number of hours of instruction required per week.

Contact Hours per Week	Credit Assigned
1 Hr. Lecture (L) per week	1 credit
1 Hr. Tutorial (T) per week	1 credit
2 Hours Practical (Lab) per week	1 credit

16. Program Structure: As per GNA University

DETAILS OF COURSES OF M.SC. PHYSICS

		Course	Credits
I.	(a)	**Core Courses (12 Subjects)**	**12 X 4 = 48**
	(b)	**Core Course Tutorial***	**12X 1 = 12**
	(c)	**Core Course Practical (9 Practicals)**	**09X 2 = 18**
II	(a)	**Elective Subjects (04)**	**4 X 4 = 16**
	(b)	**Elective Subject: Tutorial**	**4 X 1 = 4**
		Total	**98**

Semester- I

Sr. No	Course Code	Course Title	credits	L	T	P	Hours	Internal	External	Total
1	MCH1101	Organic Reaction Mechanism – I	5	4	1	0	5	40	60	100
2	MCH1102	Physical Chemistry – Thermodynamics	5	4	1	0	5	40	60	100
3	MCH1104	Computer for Chemists – Theory	4	3	1	0	4	40	60	100
4	MCH1105	Inorganic Chemistry – I	5	4	1	0	5	40	60	100
5	MCH1201	Organic Chemistry Laboratory – I	2	0	0	4	4	30	20	50
6	MCH1202	Inorganic Chemistry Laboratory – I	2	0	0	4	4	30	20	50
7	MCH1203	Computer for Chemists – Laboratory	1	0	0	2	2	30	20	50

Semester- II

Sr. No	Course Code	Course Title	credits	L	T	P	Hours	Internal	External	Total
1	MCH2105	Organometallics Chemistry	5	4	1	0	5	40	60	100
2	MCH2106	Organic Reaction Mechanism – II	5	4	1	0	5	40	60	100
3	MCH2107	Surface and Polymer Chemistry	5	4	1	0	5	40	60	100
4	MCH2108	Physical Chemistry – Quantum Chemistry	5	4	1	0	5	40	60	100
5	MCH2201	Organic Chemistry Laboratory – II	2	0	0	4	4	30	20	50
6	MCH2203	Physical Chemistry Laboratory – I	2	0	0	4	4	30	20	50

Semester- III

Sr. No	Course Code	Course Title	credits	L	T	P	Hours	Internal	External	Total
1	MCH3123	Inorganic Chemistry – II	5	4	1	0	5	40	60	100
2	MCH3110	Organic Synthesis	5	4	1	0	5	40	60	100
3		Elective – 1	5	4	1	0	5	40	60	100
4		Elective – 2	5	4	1	0	5	40	60	100
5	MCH3202	Inorganic Chemistry Laboratory – II	2	0	0	4	4	30	20	50
6	MCH3203	Physical Chemistry Laboratory – II	2	0	0	4	4	30	20	50

Semester- IV

Sr. No	Course Code	Course Title	credits	L	T	P	Hours	Internal	External	Total
1	MCH4113	Natural Products in Chemistry	5	4	1	0	5	40	60	100
2	MCH4112	Chemistry of Materials	5	4	1	0	5	40	60	100
3		Elective – 3	5	4	1	0	5	40	60	100
4		Elective – 4	5	4	1	0	5	40	60	100
5	MCH4201	Advanced Organic Chemistry Laboratory	2	0	0	2	4	30	20	50
6	MCH4202	Advanced in organic Chemistry Laboratory	2	0	0	2	4	30	20	50
7	MCH4203	Advanced Physical Chemistry Laboratory	2	0	0	2	4	30	20	50

Semester- I

Sr. No	Course Code	Course Title	credits	L	T	P	Hours	Internal	External	Total
1	MCH3125	Spectroscopy A: Techniques for Structure Elucidation of Organic Compounds	5	4	1	0	5	40	60	100
2	MCH3111	Spectroscopy B: Techniques for Structure Elucidation of Organic Compounds	5	4	1	0	5	40	60	100
3	MCH3112	Reaction Mechanisms and Metal Clusters	5	4	1	0	5	40	60	100
4	MCH3113	Ligand Field Theory	5	4	1	0	5	40	60	100
5	MCH3114	Mathematics for Chemists	5	4	1	0	5	40	60	100
6	MCH3115	Biology for Chemists	5	4	1	0	5	40	60	100
7	MCH3116	Electrochemistry and Chemical Dynamics	5	4	1	0	5	40	60	100
8	MCH3117	Photochemistry and Pericyclic reactions	5	4	1	0	5	40	60	100
9	MCH3118	Medicinal Chemistry	5	4	1	0	5	40	60	100
10	MCH3119	Advanced Functional Materials	5	4	1	0	5	40	60	100
11	MCH3120	Green Chemistry	5	4	1	0	5	40	60	100
12	MCH3121	Supramolecular Chemistry	5	4	1	0	5	40	60	100
13	MCH3122	Dissertation	5	0	0	10	10	0	100	100
14	MCH3124	Bioinorganic Chemistry	5	4	1	0	5	40	60	100

17. Examination/ Evaluation System:

17.1 Internal Assessment, which includes attendance, mid semester examination and other components (Project 1, Project 2, Mid Term Exam, Attendance, Class Test) carrying a weightage of 40%. This is applicable for all theory courses.

17.2 Practical Courses: The examination/evaluation criteria of the practical courses shall be decided by the respective faculty member and wherever required on the availability of the external experts/visiting faculty. Faculty may set/design the practical exercises out of any marks but the overall weightage shall be in pre-defined percentage, which the concerned

faculty/course coordinator shall announce in the first class of the semester and upload on the GU-MS. Methodology for evaluation of Lab component may include day to day work, lab records, quantity/quality of work and Viva/Seminar/Practical as may be decided.

17.3 External Assessment i.e. End Semester Examination, carrying a weightage of 60%.

a) **End Semester Examination:** These examinations shall be conducted by Controller of Examination. The examination dates and schedule shall be released by the University.

b) Similar division of marks may be created for special courses like Major Projects, seminars, term papers, internship etc. by respective faculty but same shall also be predefined.

c) Every student has to score at least 25% marks each in Continuous Assessment and End Semester examination. The minimum pass percentage is 40% in aggregate. In case a student scores more than 25% each in Continuous Assessment and End Semester Examination, but overall percentage in the concerned subject remains less than 40%, then student has to repeat End Semester Examination in that subject.

17.4 Failing to meet Attendance Requirement:

a) A student is required to attend all the classes.

b) If the attendance profile of a student is unsatisfactory, he/she will be debarred. Any student, who has been debarred due to attendance shortage, shall not be allowed to take the supplementary Examination. The student shall have to register for the course in the regular semester when offered.

17.5 Makeup Examinations for Mid Semester Examination: A student may apply for a makeup examination where he/she is not able to attend the examination schedule due to reasons of personal medical condition or compassionate reason like death of a very close relative. No other contingencies are acceptable. Except in case of medical emergency, a student needs to seek advance approval from appropriate authority before missing the Examination.

Theory Courses:

- A student missing Mid Term Examination only shall be required to take a make-up Examination.
- The students must put-up the request for make-up Examination along with the medical documents to prove the genuineness of the case (for having missed the Examination) within 5 days of last date of Examination.

- The genuineness shall be reviewed and approved by the Vice Chancellor, whose decision shall be final.

In case a student misses the make-up Examination also, then no further chance will be provided.

- The duration of Examination shall be as decided by the Faculty member.
- Genuine approved cases shall be notified by the Controller of Examination based on the requests received and only such students shall be allowed to take make-up Examination in the subjects where approval has been granted.
- The date sheet need not be taken out as the makeup examination shall be conducted under arrangement concerned faculty, who after evaluation and sharing the evaluated answer sheet with student shall submit marks to the Controller of Examination.

17.6 Makeup of End Semester Examination: It is mandatory to appear the end semester major examination to obtain any grade for a course. A student who misses the end semester major examination shall follow a similar procedure as outlined above, to obtain approval of the Vice Chancellor to prove genuineness of the case. The student whose case is approved as genuine shall be awarded "I" Grade in the semester results in the given subject. The student shall be allowed to appear in the supplementary examination of the said subject. However, the grades shall be worked out by computing the marks obtained by students in Mid Term Exams, TA, Lab and supplementary examination (equated to the weightage of end semester examination). The total marks shall be compared with the marks of the class as in the regular semester for award of grade.

17.7 Makeup of End Semester Viva of Projects: It is mandatory to appear in the final Viva examination to obtain any grade for a project course. In case of student missing the same for genuine reasons; similar method as given for written examination of theory courses shall be followed.

17.8 Procedure to be adopted by students in case of missing any of the specified Examination(s): Following procedure shall be adopted for establishing genuineness of the case.

a. Action by the student (Medical Cases)

I. They should report absence from the Examination(s) by fastest possible means to the Controller of Examination. It could be email or written communication by speed post or sent by hand through any means. In case of Hosteller's, if a student falls sick while residing in the hostel, he/she should seek advice of the available qualified doctor.

II. The said report should preferably be sent prior to the Examination, but not later than 5 days after the last date of the said Examination.

III. The student should on rejoining:

a. Report to the Controller of Examination with complete medical documents to include referral/Prescription slip of the doctor specifically indicating the disease and medicine prescribed, investigation/Lab reports and discharge slip in case of admission should be provided.

b. Submit the Documents to the Controller of Examination, not later than 5 days after the last date of Examination

IV. In case delay beyond 5 days is anticipated the student should arrange for the medical documents to be sent to the University Medical Officer by hand through a friend / relative etc. and get the said genuineness deposit with the Controller of Examination.

V. No request later than 5 days after the last date of Examination shall be accepted for reasons of ignorance or any other reasons.

b. Action by students (any other reason)

In case the student must miss Examination due to genuine reason other than medical, prior written sanction of Vice Chancellor and in his absence Dean is mandatory. No post facto requests shall be accepted in any case. The approval should be deposited with the Controller of Examination before the examination.

18. Supplementary Examination:

18.1 The supplementary examinations shall be held for each commiserating semester in December for Odd semester and May/June for Even semester respectively. For the final semester students, there is privilege to appear in the supplementary exams of all previous semester.

18.2 Eligibility: Student with 'F' grade is eligible to appear in the Supplementary Examination.

18.3 Re-appear: Student with backlog of one semester will be carried forward to next semester. Re-appear examinations will be conducted twice in a year after ESE of every semester.

18.4 Supplementary for Projects: There shall be no supplementary examinations for the projects, except makeup examination for missing the final viva as per rules outlined above.

19. Grading System: University follows eight letter grading system (A+, A, B+, B, C+, C, D, and F) that have grade points with values distributed on a 10 point scale for evaluating the performance of student. The letter grades and the corresponding grade points on the 10-point scale are as given in the table below. If number of passing students in any subject is less than or equal to 30 then Absolute Grading System will be followed otherwise Relative Grading System will be followed for evaluation.

Academic Performance	**Range of Marks**	**Grades**	**Grades Points**	**Remarks**
Outstanding	≥90	A+	10	
Excellent	≥80 & <90	A	9	
Very Good	≥70 & <80	B+	8	
Good	≥60 & <70	B	7	
Fair	≥50 & <60	C+	6	
Average	≥40 & <50	C	5	
Minimally Acceptable	40	D	4	
Fail	<40	F	0	
Incomplete		I	-	
Withdrawal		W	-	
Grade Awaited		GA	-	
Minor Project		**S/US**		**S-Satisfactory US-Unsatisfactory**

19.1 Description of Grades:

A. **<u>D Grade:</u>** The D grade stands for marginal performance, i.e. it is the minimum passing grade in any course. D grade shall not be awarded below 30% marks, though each teacher may set higher marks for the same.

B. **<u>F Grade:</u>** The 'F' grade denotes a very poor performance, i.e. failing a course. A student has to repeat all courses in which she/he obtains 'F' grade until a passing grade is obtained. In the case of 'F', no Grade points are awarded. However, the credits of such courses shall be used as the denominator for calculation of GPA or CGPA.

<u>W Grade:</u> The 'W' grade is awarded to a student if he/she is allowed to withdraw for an entire Semester from the University on medical grounds for a period exceeding five weeks.

<u>D. I" Grade:</u> The 'I' grade is awarded when the student is allowed additional opportunity like makeup Examination etc. based on which the grade is to be decided along with other components of the evaluation during the semester 24 An incomplete grade of 'I' may be given when an unforeseen emergency prevents a student from completing the work in a course. The 'I' must be converted to a performance grade (A to F) within 90 days after the first day of classes in the subsequent regular semester.

<u>E. X Grade:</u> It is equivalent to Fail grade but awarded due to a student falling below the laid down attendance requirement. Students having X grade shall be required to re-register for the course, when offered next.

19.2 Cumulative Grade Point Average (CGPA), it is a measure of the overall cumulative performance of a student for all semesters. The CGPA is the ratio of total credit points secured by a student in various courses in all semesters and the sum of the total credits of all courses in all the semesters. It is expressed up to two decimals places.

NB: The CGPA can be converted to percentage by using the given formula:

CGPA x 10 = %

e.g. 7.8 x 10 = 78%

19.3 Based on the grades earned, a grade certificate shall be issued to all the registered students after every semester. The grade certificate will display the course details (Course title, number of credits, grade secured) along with SGPA of that semester and CGPA earned till that semester.

20. General Rules: Examinations:

a) Showing the Answer Scripts: The answer scripts of all written Examinations i.e. Mid Term or end semester examination or any other written work conducted by a teacher shall be shown to the students. Students desirous of seeing the marked answer scripts of End Semester Examination has to ensure their presence before results are declared, as per dates notified by the Controller of Examination.

b) Marks/Answer Sheets of all other tests shall also be shared with the students and thus, there shall be no scrutiny of grades. However, before the grades are forwarded to Registrar/Controller of Examination, they should be displayed on GU-MS and time are given to students, to discuss the same with respective faculty.

c) No appeal shall be accepted for scrutiny of grades.

d) Examination Fee for Supplementary. A fee of Rs.1000/- per course or as decided by the Management from time to time will be charged from the students.

21. Program qualifying criteria: For qualifying the Program every student is required to earn minimum credits. If any student fails to earn minimum credits i.e. 98 for the program, then he/she will get a chance to complete his/her Program in two more years than the actual duration of degree.

22. Improvement of overall Score: A candidate having CGPA < 5.5 and wishes to improve his/her overall score may do so within two academic years immediately after passing the degree program by reappearing into maximum four course(s)/subject(s). The improvement would be considered if and only if the CGPA becomes > 5.5.

23. Program qualifying criteria: For qualifying the Program every student is required to earn prescribed credits (i.e. 98) If any student fails to earn prescribed credits for the program then he/she will get a chance to complete his/her Program in two more years than the actual duration of degree.

24. Revision of Regulations, Curriculum and Syllabi: The University may revise, amend, change, or update the Regulations, Curriculum, Syllabus and Scheme of examinations through the Board of Studies and the Academic Council as and when required.

25. Conditions for Award of a Degree: Should complete the requirements of the Degree in maximum duration specified for the program. Semester withdrawals due to medical reasons are not counted in six years. However, forced withdrawal of students e.g. rustication or expulsion or nonattendance by student due to any other reasons, shall count in the maximum period of six years and minimum period of four years.

GNA UNIVERSITY
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Syllabus

MASTER OF SCIENCE : CHEMISTRY

SEMESTER - I

MCH1101: Organic Reaction Mechanism-I
Credit : 05
LTP 410

Course Description:

This course deals with nature of bonding in organic reaction, stereochemistry, reaction mechanism, aliphatic nucleophilic substitution, aliphatic electrophilic substitution, aromatic nucleophilic substitution and aromatic electrophilic substitution.

Course learning outcomes: After completion of this course, students will be able to:

CO1: Distinguish between aromatic, antiaromatic and homoaromatic compounds.

CO2: Know about chiral and achiral compounds and their synthesis.

CO3: Have knowledge about reaction mechanism (kinetics and thermodynamics) and intermediates produced.

CO4: To get detailed knowledge about nucleophilic and electrophilic substitution reactions.

Course content:

Unit I

1. Nature of Bonding in Organic Reactions:

Aromaticity in Benzenoid and non-benzenoid compounds. Huckel's Rule, alternant, and non-alternant hydrocarbons. Energy levels of π (pi) molecular orbitals in simple systems. annulenes, antiaromaticity, homoaromaticity, PMO approach.

2. Stereochemistry: (8 Hrs.)

Elements of symmetry, chirality, molecules with more than one chiral center. Threo and erythroisomers, methods of resolution, optical purity. Prochirality–enantiotopic and diastereotopic atoms, groups and faces. Stereospecific and stereoselective synthesis. Asymmetric synthesis. Optical activity in absence of chiral carbon (biphenyls, allenes, spiranes). Chirality due to helical shape.

Unit II

3. Reaction Mechanism, Structure and Reactivity:

Types of mechanisms, types of reactions, thermodynamic and kinetic requirements, kinetic and thermodynamic control in product formation. Transition states and reaction intermediates, isotope effects, Hard and Soft Acid Base concept, Study of reactive intermediates–Types of intermediates, isolation and detection of intermediates (including use of spectral techniques), trapping of intermediates.

4. Aliphatic Nucleophilic Substitution:

The SN2, SN1 and SNi mechanisms, mixed SN1 & SN2mechanism, SET mechanism. The neighbouring group mechanism (anchimeric assistance). Neighbouring group participation by π and sigma bonds**.**

Unit III

5. Aliphatic Nucleophilic Substitution –

Classical, non-classical & phenonium cations, rearrangements in carbocations (general survey). Ester hydrolysis, nucleophilic substitution at allylic, aliphatic trigonal and vinylic carbon. Effect on the reactivity due to – substrate structure, attacking nucleophile, leaving group and reaction medium. Ambident nucleophiles and substrates, regioselectivity. Meyer's synthesis of aldehydes, ketones, acids and esters. Alkylation by organoboranes.

6. Aliphatic Electrophilic Substituion:

Bimolecular mechanism – SE2 and SEi. The SE1 mechanism, hydrogen exchange, electrophilic substitution accompained by double bond shifts, diazo-transfer reaction, formation of sulphur ylides, effect of substrates, leaving group and solvent polarity on the reactivity.

Unit IV

7. Aromatic Electrophilic Substitution:

The arenium ion mechanism, orientation and reactivity in mono substituted and di substituted aromatics. Energy profile diagrams. The ortho/para ratio, ipso attack, orientation in other ring systems. Quantitative treatment of reactivity in substrates and electrophiles. Diazo coupling, Vilsmeir reaction, Gattermann-Koch reaction, Pechmann reaction, Houben–Hoesch reaction, Fries rearrangement.

8. Aromatic Nucleophilic Substitution:

SNAr, SN1, benzyne and SRN1 mechanisms. Reactivity effect of substrate structure, leaving group and nucleophile. The von Richter, Sommelet-Hauser, and Smiles rearrangements.

Books Recommended:

1. Stereochemistry - Eliel
2. Advanced Organic Chemistry – Jerry March.
3. Advanced Organic Chemistry, F. A. Carey, R. J. Sundberg, Volume I and II
4. Highlights of Organic Chemistry, W.J. L. Nobel; An Advanced Text Book.
5. Stereochemistry conformation and Mechanism – P. S.

MCH1102: Physical Chemistry – Thermodynamics

Credits : 05

LTP 410

Course Description:

This course deals with classical thermodynamics, non-ideal systems, statistical thermodynamics, partition functions and non-equilibrium thermodynamics.

Course learning outcomes: After completion of this course, students will be able to:

CO1: have idea about various thermodynamic parameters for ideal and non-ideal systems.

CO2: distinguish between different statistics.

CO3: to get knowledge about the terms like ensembles, partition functions and irreversible thermodynamics.

CO4: to get knowledge about the reversible thermodynamics in biological systems.

Course content:

Unit I

1. Classical Thermodynamics

Brief resume of concepts of thermodynamics, free energy, chemical potential and entropy. Partial molar properties, partial molar free energy, partial molar volume and partial molar heat content and their significance. Determination of these quantities. Concept of fugacity and determination of fugacity.

Unit II

2. Non-ideal systems

Excess functions for non-ideal solutions. Activity, activity coefficients, Debye-Huckel theory for activity coefficient of electrolytic solutions, determination of activity and activity coefficients, ionic strength. Application of phase rule to three component system, second order phase transitions.

3. Statistical Thermodynamics

Concept of distribution law, thermodynamic probability and most probable distribution, Ensemble averaging, postulates of ensemble averaging. Canonical, grand canonical and microcanonical ensembles, corresponding distribution laws (using Lagrange's method of undetermined multipliers).

Unit III

4. Partition functions

Translational, rotational, vibrational and electronic partition function, calculation of thermodynamic properties in terms of partition functions. Application of partition functions. Heat capacity behaviour of solids-chemical equilibria and equilibrium constants in terms of partition functions, Fermi-Dirac statistics, distribution laws, and application to metals. Bose-Einstein statistics-distribution law and application to helium.

Unit IV

5. Non Equilibrium Thermodynamics

Thermodynamic criteria for non-equilibrium states, entropy production and entropy flow, entropy balance equations for different irreversible processes (e.g., heat flow, chemical reaction etc.) transformations of generalized fluxes and forces, non-equilibrium stationery states, phenomenological equations, microscopic reversibility and Onsager's reciprocity relations, electro kinetic phenomena, diffusion, electric conduction, irreversible thermodynamics for biological systems, coupled reactions.

Books recommended:

1. I F Nash: Elements of classical and statistical thermodynamics
2. Lee Bot: Irreversible thermodynamics
3. Thermodynamics of Biological Processes, D. Jou and J.E. Lee Bot
4. I Prigogine: Introduction to thermodynamics of irreversible processes
5. T L Hill: Introduction to statistical thermodynamics.

MCH1104: Computer for Chemists

Credits : 04

LTP 310

Course Description:

This course deals with basic programming, different functions, operators and arrays used in a C-program.

Course learning outcomes: After completion of this course, students will be able to:

CO1: use different operators and functions in a program.

CO2: to know floating point numbers.

CO3: to apply different types of statements and loops in routine.

CO4: to use arrays in a program.

Unit I

Principles of programming, algorithms, and flowcharts, basic structure of C program. introduction of declaration of variables, rules for naming variables, all data types, introduction to operators and its types, relative priority of arithmetic operators, use of parenthesis**.**

Unit II

Floating point numbers, scientific notation, converting integers to floating point and vice versa, coercion and cast operator, type char. Type char and ASCII code, character strings and how to print them, octal and hexadecimal notation.

Unit III

Decision making in C: if statement, if else statement, nesting of if statement.

Looping statements: while loop, do while loop, for loop, nesting of for loop, break and continue statement.

Unit IV

Arrays, declaring an array, initializing an array, strings, and character arrays, sorting an array, finding maximum and minimum in an array, multidimensional arrays.

User defined functions, returning value from a function, functions with more than one parameter.

MCH1105: Inorganic Chemistry-I

Credits : 05

LTP 410

Course Description:

This course deal with fundamental Inorganic chemistry, limitations of different theories, and concept of mechanism of inorganic reaction, thermodynamic and kinetic applications of different theories in transition metal complexes.

Course learning outcomes: After completion of this course, students will be able to:

CO1: To get knowledge about fundamental concepts of Inorganic Chemistry and their applications.

CO2: To know the limitations of different theories in different type of inorganic compounds.

CO3: To get knowledge about different type of reaction mechanisms in Inorganic Chemistry.

CO4: To get knowledge about trans effect and substitution reactions in different type of complexes.

Unit I

Stereochemistry and bonding in main group compounds, VSEPR, Walsh diagrams (tri and tetra-molecules), dπ-pπ bonds, Bent rule and energetics of hybridization, some simple reactions of covalently bonded molecules.

Unit II

Limitations of crystal field theory, molecular orbital theory, octahedral, tetrahedral and square planar complexes, π bonding and molecular orbital theory.

Unit III

Metal-Ligand equilibria in solution, stepwise and overall formation constant and their interaction, trends in stepwise constants, factors affecting the stability of metal complexes with reference to the nature of metal ion and ligand, chelate effect and its thermodynamic origin, determination of binary formation constants by pH spectrophotometry. Reaction mechanism of transition metal complexes- energy profile of a reaction, reactivity of metal complexes, inert and labile complexes, kinetic application of valance bond and crystal field theories, kinetics of octahedral substitution.

Unit IV

Reaction mechanism of transition metal complexes –II, acid hydrolysis, factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism, direct and indirect evidence in favour of conjugate mechanism, and reactions without metal-ligand bond cleavage. Substitution reactions in square planar complexes, the trans effect, mechanism of substitution reaction, Redox reactions, electron transfer reactions, mechanism of one electron transfer reactions, outer sphere type reactions, cross reactions and Marcus Hush Theory, inner sphere type reactions.

Books Recommended

1. Cotton, F.A.; Wilkinson Advanced Inorganic Chemistry, 6th edition, John Wiley& Sons, 1999.
2. Huheey, James E. Inorganic Chemistry: Principles of Structure and Reactivity, 4 th edition, Harper Collins College Publishers, 1993.
3. Greenwood, N.N. and Earnshaw, A. Chemistry of the Elements, 2nd edition, Butterworth Heinemann, A division of Read Educational & Professional Publishing Ltd., 2001.
4. Lever, A.B.P. Inorganic Electronic Spectroscopy, 2nd edition, Elsevier Science Publishers B.V., 1984.
5. Carlin, Richard L. and Duyneveldt, A.J.Van Magnetic Properties of Transition Metal Compounds, Inorganic Chemistry Concepts 2, Springer-verlag New York Inc., 1977.
6. Shriver, D.F.; Atkins, P.W. Inorganic Chemistry, 1st edition, Oxford University Press, 2006.
7. Drago, Russell S. Physical Methods for Chemists, 2nd edition, Saunders College Publishing, 1992.

MCH1201: ORGANIC CHEMISTRY LABORATORY-I

Credits : 02

LTP 002

Course Objectives:

This course deals with purification and characterization of organic compounds, thin layer chromatography, organic synthesis and extraction of organic compounds.

Course learning outcomes: After completion of this course, students will be able to:

CO1: perform different techniques of separation and confirm it by TLC.

Co2: to synthesize different organic compounds and extract caffeine and casein.

Course content:

1. Purification and Characterization of Organic Compounds, (i) the student is expected to carry out the experiments of purification (fractional crystallization, fractional distillation, chromatography) separation, purification and identification of the compounds of binary organic mixture (liquid-liquid, liquid-solid and solid-solid), using chemical analysis and IR and PMR spectral data. The student should also check the purity of the separated components on TLC plates.

(ii) To carry out the analysis of common analgesic drugs by thin layer chromatography, Acetaminophen, Aspirin, caffeine, phenacetin, salicylamide. (Learn to check purity of the given samples and completion of the chemical reactions).

2. Organic Synthesis and Extraction of Organic Compounds from Natural Sources. The student is expected to carry out 4 to 6 organic preparations (usually involving not more than two steps), some of the illustrative experiments are listed below:-

1. Extraction of Caffeine from tea leaves

(Ref. Experiment Organic Chemistry, (H. Dupont Durst, George W. Gokel, P 464 McGraw Hill Book Co., New York).

Student would be asked to purity crude sample, check the purity on a TLC single spot and get the NMR scanned and interpret (Three methyl singlets and I methane singlet).

2. *Isolation of casein from milk* **(try some typical colour reactions proteins).**

3. *Synthesis of 2-phenylIndole-Fischer Indole Synthesis.* Book 1, p. 852

Aim: To Study condensation and cyclization reactions.

4. *Synthesis of 3-nitrobenzoic from benzoic acid* (Rf. Ibid., p.245-247 and 443-448).

Aim: To demonstrate the process of meta nitration, esterification and saponification of an ester. Make a comparative study of IR and PMR spectra of benzoic acid, methyl benzoate, methyl 3-nitrobenzoate.

5. *Cannizaro's reaction of 4-chlorobenzaldehyde.*. Book 1, p 760

Aim: To demonstrate technique of isolation of two products from the reaction mixture and the procedure of intermolecular hydride transfer. Make a comparative study of IR and PMR spectra of 4 chlorobenzadehyde, 4-chlorobenzoicacid 4-chlorobenzyl alcohol.

6. *Synthesis of 1,3,5-Tribromobenzene from aniline.*

Aim: To demonstrate: Bromination, Diazotization and Reduction.

Book recommended:

Vogel's Text book of practical organic chemistry, 5th edition.

MCH1202: INORGANIC CHEMISTY LABORATORY-I

Credits : 02

LTP 002

Course Objectives:

This course deals with oxidation-reduction titrations, precipitation titrations, complexometric titrations and gravimetric analysis.

Course learning outcomes: After completion of this course, students will be able to:

CO1: perform different techniques of separation and confirm it by TLC.

CO2: use gravimetric analysis for estimations of different metal ions.

Course content:

I. Oxidation-Reduction Titrations

1. Standardization with sodium oxalate of $KMnO_4$ and determination of Ca^{2+} ion.
2. Standardization of ceric sulphate with Mohr's salt and determination of NO_3^{-1} and $C_2O_4^{2-}$ ions.
3. Standardization of $K_2Cr_2O_7$ with Fe^{2+} and determination of Fe^{3+} (Ferric alum)
4. Standardization of hypo solution with potassium iodate / $K_2Cr_2O_7$ and determination of available Cl_2 in bleaching powder, Sb^{3+} and Cu^{2+}.
5. Determination of hydrazine with KIO_3 titration.

II. Precipitation Titrations

1. $AgNO_3$ standardization by Mohr's method by using adsorption indicator.
2. Volhard's method for Cl^- determination.
3. Determination of ammonium / potassium thiocyanate.

III. Complexometric Titrations

1. Determination of Mg^{2+} and Mn^{2+} in a mixture using fluoride ion as a demasking agent.
2. Determination of Ni^{2+} (back titration).
3. Determination of Ca^{2+} (by substitution method).

IV. Gravimetric Analysis

1. Determination of Ba^{2+} as its chromate.
2. Estimation of lead as its lead molybdate.
3. Estimation of chromium (III) as its lead chromate.

4. Estimation of Cu2+ using Ammonium/ Sodium thiocyanate.

Books recommended:

Vogel's book on Inorganic Quantitative Analysis.

MCH1203: Computer programs in Chemistry

Credits : 01

LTP 001

Course Description:

Development of small computer codes involving simple formulae in chemistry.

Course learning outcomes: After completion of this course, students will be able to:

CO1: perform different techniques of separation and confirm it by TLC.

CO2: use gravimetric analysis for estimations of different metal ions.

Course content:

Unit I

1. Calculation of simple interest.
2. Find the largest number out of any given three numbers.
3. Write a program to show the purpose of switch statement.
4. Calculate sum of digits of a given number.
5. Write a program to describe the input output in array.
6. Write a program to find the factorial of a number.

Unit II

7. Calculation of Bohr orbit from de Broglie Lambda for electron.
8. Calculation of wave number and frequency from value of wave length.
9. Calculation of van der Waals radii.
10. Compute the Radioactive decay constant.
11. Rate constant of a 1st order reaction, 2nd order reaction.
12. Calculation of lattice energy using Born Lande equation.

Unit III

13. Addition, multiplication and solution of inverse of 3 X 3 matrix.
14. Calculation of average molecular weight of a polymer containing n1 molecules of molecular weight M1, n2 molecules of molecular weight M2 and so on.
15. Program for calculation of molecular weight of organic compound containing C, H, N, O and S.
16. Calculation of reduced mass of diatomic molecule.
17. Calculate the RMS and most probable velocity of a gas.

Unit IV

18. Calculate the ionic mobility from ionic conductance values.

19. Determine the thermodynamic parameters for isothermal expansion of monoatomic ideal gas.

20. Calculate the bond length and bond angles using crystal structure data

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Books recommended:

1. K.V. Raman, Computers in Chemistry, Tata McGraw Hill.

2. Mullish Cooper, The spirit of c, An Introduction to Modern Programming.

3. Pundir-Bansal, Computers for Chemist, Pragati Prakashan Meerut

MCH2105: ORGANOMETALLICS CHEMISTRY

Credits : 05

LTP: 410

Course Description:

This course deals with organometallics, reaction at coordinated ligands, homogeneous hydrogenation, metal carbonyls and acceptor character of CO2, O2, N2, Ph3.

Course learning outcomes: After completion of this course, students will be able to:

CO1: learn about the synthesis methods of organometallic compounds and heptacity.

CO2: to carry out different chemical modifications at the coordinated ligands.

Co3: to learn about the complexes formed by ligands with п-character.

CO4: to learn different reactions of metal carbonyls with different ligands.

Course content:

Unit I

1. Organometallics:

Energy polarity and reactivity of M-C bond, Stability of main group organometallics: Methods of preparation in perspective-organolithium compounds: structure and bonding & reaction carbolithiatic organometallics of group 2 and 12 e.g., Mg and Zn, Cd and Hg: Preparation and structure of organoaluminium compounds, technical applications of Tris (alkyl) aluminium compounds. Ƞ2–ligands: olefinic and acetylenic complexes, chelating olefinic ligands–synthesis and structure. Ƞ2–ligands: allylic and Ƞ4–complexes of cyclopentadiene.

Unit II

2. Synthesis and structure. Ƞ4 –ligands: Butadiene, cyclobutadiene, heterocyclic pentadiene (S, Se, Te). Classification, nomenclature of cyclopentadienyl complex, preparation of cyclopentadienyl

T.M. Complexes. MO treatment of ferrocene. Ƞ6–ligands: benzene and its derivatives, multidecker sandwich compounds.

3. Reaction at Coordinated ligands:

The role of metal ions in the hydrolysis of amino acid esters, peptides, and amides molecular orbital concept of role of metal ions participation, modified aldol condensation, imine formation, template and macrocyclic effect in detail.

Unit III

4. Homogeneous hydrogenation of unsaturated compounds, reversible cis-dihydrocatalysis, monohydrido compounds, asymmetrical hydrogenation, hydrosilation of unsaturated compounds, hydrocyanation of alkenes, alkane metathesis, Ziegler-Natta polymerization of ethylene and propylene, water gas shift reaction, acetic acid synthesis by carbonyls, oxopalladation reactions. Organometallic reagents in organic synthesis.

Unit IV

5. π- acceptor character of CO, O_2, N_2, NO, PH_3 molecules in terms of MOEL diagram, Metal carbonyls; structure and bonding; vibration spectra of metal carbonyls for bonding and structural elucidation, important reactions of metal carbonyls; preparation, bonding structure and important reactions of transition metal nitrosyl, dinitrogen and dioxygen complexes; tertiary phosphine as ligand.

Books Recommended:

1. C. Elschenbroich and A. Salzer, Organometallics: A Concise Introduction, 2nd Ed., VCH 1992.
2. J.E. Huheey, Inorganic Chemistry Principles of Structure and Reactivity, Harper Interscience.
3. F.A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, Ed. V & VI. Wiley Interscience.
4. G. L. Miessler, D. A. Tarr, Inorganic Chemistry, 3rd edition, Pearson Education

MCH2106: Organic Reaction Mechanism–II

Credits : 05

LTP 410

Course Description:

This course deals with free radical reactions, elimination reactions, carbon multiple bonds, hetero multiple bonds, formation of carbon-carbon bond, oxidation and reduction.

Course learning outcomes: After completion of this course, students will be able to:

CO1: distinguish between free radical, elimination and addition reactions.

CO2: learn about organic synthesis involving formation of new C-C bond.

CO3: have an idea about reactions of aldehydes and ketones and different named reactions.

CO4: To learn about different oxidising and reducing reagents

Course content:

Unit I

1. Free Radical Reactions

Types of free radial reactions, free radical substitution mechanism. Mechanism at an aromatic substrate, neighbouring group assistance. Reactivity for aliphatic and aromatic substrates at a bridge head. Reactivity in the attacking radicals. Effect of solvents on reactivity. Allylic halogenation (NBS), oxidation of aldehydes to acids, auto-oxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salts. Sandmeyer reaction, Free radical rearrangement, Hunsdiecker reaction, Kolbe reaction, Hydroxylation of aromatics by Fenton's reagent.

2. Elimination Reactions

The E2, E1, E1cB mechanisms. Orientation of the double bond. Effects of substrate structure, attacking base, leaving group and medium on reactivity. Mechanism and orientation in pyrolytic limitations.

Unit II

3. Addition to Carbon – Carbon Multiple Bonds

Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, regio- and chemo-selectivity, orientation and reactivity. Addition to cyclopropane ring. Hydroboration, Michael reaction. Sharpless asymmetric epoxidation, hydrogenation of double and triple bonds. Hydrogenation of aromatic rings.

4. Addition to Carbon – Hetero Multiple Bonds

Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acids, esters and nitriles, Wittig reaction.

Unit III

5. Addition to Carbon – Hetero Multiple Bonds

Mechanism of condensation reactions involving enolates – Aldol, Knoevenagel, Claisen, Mannich, Benzoin, Perkin and Stobbe reactions, Reformatski reaction.

6. Formation of Carbon-Carbon Bond

Principle, disconnections and synthons, electrophilic and nucleophilic carbon species. Base catalyzed condensations; Aldol condensation, Claisen reaction, Perkin reaction, Stobbe condensation, Darzen condensation, Knoevengal reaction, Use of malonic, acetoacetic and cyanoacetic esters, Micheal addition, Wittig reactions. Use of acetylides, Acid-catalyzed condensation–self condensation of olefins, Friedal-Craft's reactions, Fries reactions, Mannich reaction, Mannich bases as intermediates in organic synthesis. Four centre reactions. Diels-Alder reaction, 1-3 Dipolar additions.

Unit IV

7. Oxidation

Introduction. Different oxidative processes. Hydrocarbons - alkenes, aromatic rings, saturated CH groups (activated and unactivated). Alcohols, diols, aldehydes, ketones, ketals and carboxylic acids. Amines, hydrazines, and sulphides. Oxidations with ruthenium tetraoxide, iodobenzene diacetate and thallium (III) nitrate.

8. Reduction

Introduction, different reductive processes, hydrocarbons-alkanes, alkenes, alkynes and aromatic rings. Carbonyl compounds – aldehydes, ketones, acids and their derivatives. Epoxides. Nitro, nitroso, azo and oxime groups. Hydrogenolysis.

Books Recommended:

1. Principles of Organic Synthesis – Norman and Coxon
2. Advanced Organic Chemistry – JerryMarch.
3. Advanced Organic Chemistry, F.A. Carey, R.J. Sunberg.
4. Highlights of Organic Chemistry, W, J.L. Nobel; An Advanced Text Book.

5. Hand Book of Reagents for Organic Synthesis - Oxidizing and Reducing Reagents. S. D. Burke and R. L. Danheiser (John Wiley and Sons)
6. Organic Synthetic reactions by William Carruthers

MCH2107: SURFACE AND POLYMER CHEMISTRY

Credits : 05

LTP 410

Course Description:

This course deals with concepts involving absorption, micelles, macromolecules, kinetics of polymerization.

Course learning outcomes: After completion of this course, students will be able to:

CO1: learn about various adsorption phenomena and micelle formation.

CO2: have knowledge about basics of polymers and their molecular weight determination.

CO3: learn about osmometry, viscometry, and diffusion.

CO4: have an idea about thermodynamics and kinetics of polymerization.

Course content:

Unit I

1. Adsorption

Surface tension, capillary action, pressure difference across curved surface (Laplace equations), vapor pressure of droplets (Kelvin equation), Gibbs adsorption isotherm, estimation of surface area (BET equation), surface films on liquids (Electro-kinetic phenomena), catalytic activity at surfaces.

Unit II

2. Micelles

Surface active agents, classification of surface active agents, micellization, hydrophobic interactions, critical micellar concentration (CMC), factors affecting CMC of surfactants, counter ion binding to micelles, thermodynamics of micellization – phase separation and mass action models, solubilization, micro emulsion, reverse micelles.

Unit III

3. Macromolecules

(a) Polymer – definition, types of polymers, electrically conducting, fire resistant, liquids crystal polymers, Importance of polymers, Basic concepts: monomers, repeat units, degree of polymerization. Linear, branched and network polymers. Classification of polymers. Molecular mass, number and mass average molecular mass, molecular mass determination (osmometry, viscometry, diffusion and light scattering methods), sedimentation, chain configuration of macromolecules, calculations of average dimensions of various chain structures.

Unit IV

(b) Kinetics of polymerization, Structure and Properties

Kinetics of polymerization, Polymerization: condensation, addition, radical chain-ionic and coordination and copolymerization. Polymerization conditions and polymer reactions. Polymerization in homogenous and heterogeneous systems. Number, weight and viscosity average weights. thermodynamics of polymerization. Polymer structure and properties-crystalline melting point Tm melting point of homogenous series, effect of chain flexibility and steric factors, entropy and heat of fusion. The glass transition temperature Tg, relationship between Tm and Tg, effects of molecular weight, diluents, chemical structure, chain topology, branching and chain linking. Property requirements and polymer utilization.

Books recommended:

1. Physical Chemistry, P. W. Atkins.

2. Textbook of polymer science, F. W. Billmeyer Jr. Wiley.

3. Polymer science, V. R. Gowariker, N. V. Viswanathan and J. Sreedhar, Wiley-Ea

MCH2108: Physical Chemistry–Quantum Chemistry

Credits : 05

LTP : 410

Course Description:

This course deals with quantum theory, operators and observations, applications of quantum postulates, angular momentum, general orbital theory of conjugated systems and the approximate methods.

Course learning outcomes: After completion of this course, students will be able to:

CO1: learn about introduction of quantum theory.

CO2: have knowledge about operators and eigen value equation.

CO3: have idea about general orbital theory and other concepts of quantum mechanics.

CO4: have an idea about Perturbation and Variation methods and their applications.

Course content:

Unit I

1. Quantum Theory: Introduction and Principles:

Black body radiations, Planck's radiation law, photoelectric effect, Compton effect, De-Broglie hypothesis, Heisenberg's uncertainty principle, Rydberg relation for explaining atomic spectrum of hydrogen. Bohr's Theory and its limitation solution of classical wave equation by separation of variables method.

Unit II

2. Operators and observations, normal and orthogonal functions, hermitian and unitary operators, introduction to differentiation and integration, Eigen value equation. Hamiltonian operator, interpretation of wave function, postulates of quantum mechanics.

Unit III

3. Applications of Quantum Postulates

Solution of particle in one- and three-dimensional box, degeneracy, the linear harmonic oscillator, rigid rotators, quantization of vibrational and rotational energy levels, hydrogen and hydrogen like atoms.

4. Angular Momentum

Commutative laws, need of polar coordinates, transformation of Cartesian coordinate into polar coordinate, angular momentum of one particle system, orbital angular momentum, the ladder operator method for angular momentum, spin angular momentum and their relations

Unit IV

5. General Orbital Theory of Conjugated Systems

Chemical bonding, linear combination of atomic orbital, overlap integral, coulomb's integral, bond order, charge density calculations for ethylene, allyl system, butadiene system, cyclobutadiene, cyclopropenyl system.

6. The Approximate Methods

Need for approximation methods, perturbation and variation methods and their application to helium atom.

Books recommended:

1. Physical Chemistry, A Molecular Approach by Mac Quarrie and Simon.
2. Quantum Chemistry, Ira N. Levine, Prentice Hall.
3. Quantum Chemistry, H. Eyring, Kimball and Walter.
4. Quantum Chemistry, Atkin.
5. Fundamentals of Quantum Chemistry, Anantharaman. R.

MCH2201: ORGANIC CHEMISTRY LABORAOTRY-II

Credits : 02

LTP : 002

Pre-Requisites: NA

Course Description:

This course deals with multistep organic synthesis and quantitative analysis of organic compounds.

Course learning outcomes: After completion of this course, students will be able to:

CO1: learn about applications of multistep organic synthesis.

CO2: have knowledge about quantitative analysis of organic compounds.

Course content:

I. Multistep Organic Synthesis

1. Synthesis of 2-chloro-4-bromoaniline from aniline (Bromination and chlorination) (Book 1)
2. Synthesis of methyl orange from aniline (Aromatic electrophilic substitution and diazocoupling) (Book 2, page 250).
3. Synthesis of benzpinacol and its pinacol rearrangement.
4. Synthesis of o-chlorobenzoic acid from phthalimide. Synthesis of acridone from ochlorobenzoic acid (Hofmann bromamide and Sandmeyer's reaction).
5. Synthesis of 2,4-dinitrophenyl hydrazine from chloro benzene. (Electrophilic and nucleophilic substitution reactions on aromatic ring).
6. Synthesis of triphenylcarbinol from bromobenzene. (Grignard reaction) (Book 2).

II. Quantitative Analysis of Organic Compounds:

1. Estimation of phenol/aniline using bromate-bromide solution (The application to find the purity of the sample and to determine the amount in given solution).
2. Determine the number of hydroxyl and amino groups in the given sample by the acetylation method.
3. Determine the mol. wt. of the given ketone by using 2, 4-DNPmethod.
4. Estimation of reducing sugar by Fehling solution method.
5. To determine the saponification value of the given fat or oil sample.
6. To determine the iodine number of the given fat or oil sample.

Books Recommended:

1. An Introduction to Modern Experimental Organic Chemistry, R. M. Roberts, J. C. Gilbert, L.B.Rodewald and A. S. Wingrove Holt, Ranehart and Winston Inc. New York.
2. Introduction to Organic Laboratory Techniques – A Contemporary Approach. D. L. Pavia,
3. G. M. Lampmana and G. S. Kriz, W. B. Saunders Company, 1976.
4. Laboratory Experiments in Organic Chemistry, R. Adams, J. R. Johnson and C. F. Wilcox. The Macmillan Limited, London.
5. Text Book of Practical Organic Chemistry, A. I. Vogel.

MCH2203: Physical Chemistry Laboratory-I

Credits : 02

LTP : 002

Course Objectives:

Course Description:

This course deals with pH metry, conductometry, emf measurements, surface tension, refraction, distribution law and polarimetry.

Course learning outcomes: After completion of this course, students will be able to:

CO1: use pH meter, conductometer, polarimeter and refractometer.

Co2: find out emf, surface tension and distribution constant.

Course content:

1. To determine the strength of given acid by pH metrically.
2. To determine dissociation constant of given acid pH metrically
3. Titration of weak acid conductometrically
4. Titration of strong acid conductometrically
5. To determine dissociation constant of given acid conductometrically
6. Determine the dissociation constant of acetic acid in DMSO, DMF, dioxane by titrating it with KOH.
7. Determine the activity coefficient of an electrolyte at different molalities by e.m.f. measurements.
8. Compare the cleansing powers of samples of two detergents from surface tension measurements.
9. Determine the specific refraction, molar refraction and atomic parachor with the help of Abbe's refractometer.
10. To study the distribution of benzoic acid between benzene and water.
11. Determine the equilibrium constant of reaction Kl +l2 + Kl3 by distribution law and hence find the value of GO of the above reaction.
12. Compare the relative strength of CH3COOH and ClCH2COOH from conductance measurements.
13. Determine the solubility (g/litre) of sparingly soluble lead sulphate from conductance measurements.
14. Titrate a given mixture of HCl and CH3COOH against NaOH solution conductometrically.
15. Compare the relative strength of:

I) HCl and

ii) H2SO4 by following the kinetics of inversion of cane sugar polarimetrically.

MCH3123: INORGANIC CHEMISTRY – II

Credits : 05

LTP : 410

Course Description:

This course deals with photo-inorganic chemistry, transition metal compounds with bonds to hydrogen, oxidative addition and migration, and transition metal complexes in catalysis.

Course learning outcomes: After completion of this course, students will be able to:

CO1: learn about photochemical processes and hydride complexes.

CO2: learn about the basics of photo Inorganic Chemistry.

CO3: learn about oxidative addition and migration reactions and catalytic reactions of transition metal complexes.

CO4: learn about the mechanism of different inorganic reactions and oxygen transfer reactions.

Course content:

Unit I

1. Photo Inorganic Chemistry-I

Basics of photochemistry- Absorption, excitation, photochemical laws, quantum yield, electronically excited states, life times- measurements of the times Flash photolysis, energy dissipation by radiative and non-radiative processes, absorption spectra, Franck-Condon principle, photochemical stages-primary and secondary processes, Kashia's rule, Thexi state, Photo substitution reactions, Adamson's rules, Photo substitution reactions of Cr(III)-Polypyridyls, Rh(III) Ammine Complexes, Ru-Polypyridyl complexes, Ligand photo reactions, photo redox reactions, comparison of Fe (II) and Ru (II) complexes

Unit II

2. Photo Inorganic Chemistry-II

Photo reactions and solar energy conversions, Photo synthesis in plants and Bacterio chlorophyll photosynthesis, photolysis of water using Inorganic precursors.

3. Transition Metal Compounds with Bonds to Hydrogen

Characteristics of hydride complexes, synthetic methods, chemical behaviour of hydride compounds, mononuclear polyhydrides, homoleptic polyhydride anions; carbonyl hydrides and onion. Molecular hydrogen compounds; metal hydrogen interaction with C-

bonds; MH interactions; complexes of boron hydride and alumina hydrides, synthetic applications of metal hydrides.

Unit III

4. Oxidative-Addition and Migration (Insertion Reactions)

Introduction: Acid base behaviour of metal atoms in complexes, Protonation and Lewis Base behaviour, acceptor properties of Lewis acidity of complexes, oxidative addition and reductive elimination, addition of specific molecules, Hydrogen addition, HX additions, Organic halides addition of some other molecules productive elimination, migration (Insertion) reaction promotion of alkyl migration, insertion of CO into M-H bonds, other aspects of CO insertion reactions, transfer of other molecules, CO2, SO2 , NO2 , RCM, Insertion of alkenes and C-C unsaturated compounds, Cleavage of C-H bonds; alkane activation, cyclometallation reactions. Reactions of free hydrocarbons.

Unit IV

5. Transition Metal Complexes in Catalysis

Hydroformylation of unsaturated compounds, Reductive carbonylation of alcohols and other compounds; Carbonylation Reaction: Methanol and methyl acetate, Adipic ester. Synthesis and other carbonylation reactions, decarbonylation reactions. Catalytic addition of molecules to C-C multiple bonds homogeneous hydrogenation, hydrocyanation of unsaturated compounds, hydrosilation of unsaturated compounds, hydrocyanation of alkenes, Polymerization, Oligomerisation and metathesis reactions of alkenes and alkynes, Ziegler-Natta polymerisation of ethylene and propylene oligomerisation and related reactions, Cluster compounds in catalysis, supported homogeneous and phase transfer catalysis, Oxidation reaction: Oxidative carbonylations, Palladium catalysed oxidation of ethylene, Acrylonitrile synthesis, oxygen transfer from peroxo- and oxo- species, oxygen transfer from NO2 groups.

Books Recommended:

1. Concepts of Inorganic Photochemistry, A. W. Adamson and P. D. Fleischauer, Wiley.

2. W.W. Porterfield, Inorganic Chemistry: A Unified Approach.

3. F.A. Cotton and G. Willkinson, Advanced Inorganic Chemistry, 5th ed., John Wiley &Sons, New York.

4. C. Elschenbroich and A. Salzer, Organometallics: A Concise Introduction, 2nd Ed., VCH 1992.

MCH3110: ORGANIC SYNTHESIS

Credits: 05

LTP 410

Course Description:

This course deals with rearrangements, polynuclear compounds and macro-ring compounds, heterocyclic synthesis, small ring heterocycles, six-membered heterocycles with one heteroatom, seven and large membered heterocycles and reagents in organic synthesis.

Course learning outcomes: After completion of this course, students will be able to:

CO1: get knowledge about general rearrangements and reagents used in organic chemistry.

CO2: have knowledge about polynuclear and heterocyclic compounds and their synthesis.

CO3: know the basics about supramolecular chemistry.

CO4: To learn about the different reagents and their specific chemical reactions.

Course content:

Unit I

1. Rearrangements

General mechanistic considerations – nature of migration, migratory aptitude, memory effects. A detailed study of the following rearrangements: Pinacol-pinacolone, Wagner-Merwein, Demjanov, Benzil-Benzilic acid, Favorskii, Arndt-Eistert synthesis, Neber, Beckmann, Hofmann, Curtius, Schmidt, Baeyer-Villiger, Shapiro reaction.l.

Unit II

2. Polynuclear Compounds & Macro-Ring Compounds

Introduction, comparative study of aromatic character of Linear and non-Linear-ortho-fused polynuclear hydrocarbons, ortho-and peri-fused polynuclear hydrocarbons. General method of preparation and reactions of indene, fluorene anthracene and phenanthrene. Modern methods of synthesis of macro ring compounds-civiton, muscone and catenoids.

3. Supramolecular Chemistry

Definition and development of supramolecular chemistry, Classification of supramolecular Host-Guest compounds, historical concepts such as receptors, coordination, lock and key analogy, Chelate and Macrocyclic effects, Preorganization and Complementarity, thermodynamics and kinetic selectivity, overview of intermolecular forces such as hydrogen bonding, hydrophobic effects, cation-π interactions, ion-ion, ion-dipole, dipole-dipole interactions, π-π stacking, vander Waals forces, synthesis and structure of supramolecular hosts for recognition of cations: crown ethers, cryptands, spherands, siderophores; for recognition of anions: guanidinium based receptors; for recognition of neutral molecules: cyclotriveratrylene (CTV).

Unit III

4. Heterocyclic Synthesis

Principles of heterocyclic synthesis involving cyclization reactions and cycloaddition reaction.

5. Small Ring Heterocycles

Three-membered and four-membered heterocyclic–synthesis and reactions of aziridines, oxiranes, thiiranes, azetidines, oxetanes and thietanes.

6. Six-Membered Heterocycles with one Heteroatom

Synthesis and reactions of pyrylium salts and pyrones and their comparison with pyridinium & thiopyrylium salts and pyridones.Synthesis and reactions of quinolizinium and benzopyrylium salts, coumarins and chromones.

7. Seven-and Large-Membered Heterocycles

Synthesis and reactions of azepines, oxepines, thiepines, diazepines, thiazepines, azocines, diazocines, dioxocines and dithiocines.

Unit IV

8. Reagents in Organic Synthesis

Use of the following reagents in organic synthesis and functional group transformations; Complex metal hydrides, Gilman's reagent, lithium dimethylcuprate, lithiumdisopropylamide (LDA), dicyclohexylcarbodimide. 1,3-Dithiane (reactivity umpolung), trimethylsilyl iodide, tri-n-butyltin hybride, Woodward and prevost hydroxylation, osmium tetroxide, DDQ, selenium dioxide, phase transfer catalysts, crown ethers and merrifield resin, Peterson's synthesis, Wilkinson's catalyst, Baker yeast.

Book Recommended

1. Supramolecular Chemistry, Jonathan W. Steed, Jerry L. Atwood, John Wiley & Sons

MCH3202: Inorganic Chemistry Laboratory-II

Credits: 02

LTP 002

Course Objectives:

This course deals with the synthesis of various complexes in Inorganic Chemistry, their properties and characterization.

Course learning outcomes: After completion of this course, students will be able to:

CO1: synthesize different metal ion based coordination complexes.

CO2: to study the characterization and confirmation of the complexes synthesized.

Course content:

Unit I

Recreation: Meaning, definition, aim, objective, scope, types,, Importance, Principles, significance of recreation.

Historical development of recreation in India

(Preparations)

1. Preparation of Co (acac)3, its characterization using NMR, IR, UV-Vis and analysis of Cobalt. (ref. J. Chem. Edu., 1980, 57, 7, 525)
2. Preparation of Co (acac-NO2)3, its characterization using NMR, IR, UV-Vis and analysis of Cobalt. (ref. J. Chem. Edu., 1980, 57, 7, 525)
3. Preparation of [Fe(H2O)6] [Fe(N-salicyldeneglycinato)2]2.3 H2O, its characterization using IR, UV-Vis, magnetic susceptibility and analysis of Iron. (ref. Inorganica Chimica Acta,1977, 23, 35).
4. Preparation of [Ni(NH3)6]Cl2 its characterization using IR, UV-Vis, magnetic susceptibility and analysis of Nickel and NH3. (ref. Marr and Rockett, 1972).
5. Preparation of [Ni(ethylenediamine)3]Cl2 its characterization using IR, UV-Vis, magnetic susceptibility and analysis of Nickel. (ref. Marr and Rockett, 1972, page 270).
6. Preparation of [Fe(NO)(S2CN(Et)2)2] its characterization using IR, UV-Vis, magnetic susceptibility and analysis of Fe(II). (ref. Marr and Rockett, 1972, page 262, J. Chem. Soc.1962, 84, 3404).
7. Preparation of octahedral and tetrahedral complexes of dichloro dipyridyl cobalt (II),differentiate them using IR, UV and magnetic properties. Estimate Co(II) from one of them. (ref. Marr and Rockett, 1972, page 375, Inorganic Chemistry, 1966, 5, 615).
8. Preparation of VO(acac)2 and its piperidine complex, characterize using IR, UV and magnetic moment. Estimate for V (IV). (ref. Marr and Rockett, 1972, 243).
9. Preparation of diaquo tetraacetatao copper (II), magnetic susceptibility IR and UV-Vis, analysis of Copper (II).
10. Preparation of cis- and trans- potassium dioxalato diaquochromate(III). Interpretation of IR, UV and magnetic properties. Estimation of Chromium. (ref. Marr and Rockett, 1972, page 386).
11. Preparation of HgCo(NCS)4 , its IR and measure its magnetic moment. (ref. Marr and Rockett, 1972, page 3).
12. Preparation of sodium tetrathionate, interpretation of its IR and analysis using potassium iodate. (ref. Marr and Rockett, 1972, page 214).
13. Preparation of Potassium dithionate, interpretation of its IR and analysis using potassium iodate. (ref. Marr and Rockett, 1972, page 214).
14. Preparation of bis(acetylacetonato) copper(II), UV-Vis, and IR, magnetic studies, Demonstration of Jahn Teller effect by solution spectral studies. (ref. Bull. Chem. Soc. Japan, 1965, 29, 852).
15. Preparation of salicylamide complexes of Copper (II). IR, UV, magnetic data and analysis of Cu (II). (ref. Indian J. of Chem., 1977, 15A, No. 5, 459; ibid, 1971, 9, 1396).
16. To prepare a macrocyclic ligand 5,7,7,12,14,14-hexamethyl-1,4,8,11-tetraazacyclotetradeca-4,11-dienedi(hydrogeniodide) and its complex with Ni(II). Study IR, NMR and UV-Vis of ligand and complex and magnetic properties of complex. To analyze for Ni and I. (J. Chem. Edu. 1977, 79, 581).
17. Preparation and resolution of tris(ethylenediamine) cobalt (III). UV-Vis, NMR, IR, optical rotation of the resolved complexes. (ref. Marr and Rockett, 1972, page 386).

Books recommended:

1. B.N. Figgis, Introduction to Ligand Field, Wiley Eastern.
2. A.B.P. Lever, Inorganic Electronic Spectroscopy, Elsevier.

3. A.Earnshaw, Introduction to Magnetochemistry, Academic Press.
4. J.E. Huheey, Inorganic Chemistry Principles of Structure and Reactivity, Harper Inter science.
5. R.S. Drago, Physical Medhod in Chemistry, W.B. Saunders Company.
6. F.A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, Wiley Interscience.
7. F.A. Cotton, Chemical Application of Group Theory, Wiley Eastern.

MCH3203: PHYSICAL CHEMISTY LABORAOTRY-II

Credits : 02

LTP : 002

Course Description:
This course deals with the determination of partial molar volume, surface tension, refractive index, conductance, dissociation constant and use of spectrophotometer, potentiometer and turbidity meter.

Course learning outcomes: After completion of this course, students will be able to:
CO1: learn how to find out partial molar volume, surface tension, refractive index, conductance and dissociation constant.
CO2: to use spectrophotometer, potentiometer and turbidity meter.

Course content:
1. To determine the partial molar volume of
(a) Glycine (b) Urea using dialtometer
2. To determine the partial molar volume of
(a) methanol (b) n-propanol using dilatometer
3. To determine the surface tension (double capillary) of mixture of solid and water by differential method and hence find out parachor of the mixture.
4. To determine the specific and molar refractivity of n-propanol, butanol, hexane and carbon tetrachloride and calculate refraction equivalents of C, H and Cl.
5. To determine the molar refractivity of water, DMF, Dioxane and mixtures of water, DFM, water-Dioxane and verify the refractivity rule. Predict about the interactions between components of mixture by plotting graph between refractive index and mole fraction.
6. To determine the equivalent conductance of weak electrolyte acetic at infinite dilution using Kohlrausch law.
7. Determine equivalent conductance of strong electrolyte at several concentrations and hence verify Onsagars equation.
8. Determine equivalent conductance of weak electrolyte, say, acetic acid at different concentrations and hence test validity of Oswald's dilution law. Also determine dissociation

constant of the electrolyte.

9. To determine dissociation constant of a dibasic acid potentiometrically.

10. To study complex formation between Fe (III) and salicylic acid and find out the formula of the complex spectrophotometrically.

11. To determine the formula of the complex ion formed between Fe (III) and Thiocyante ion by Job's method.

12. To study the kinetics of hydrolysis of crystal violet spectrophotometrically.

13. To determine the pH of a buffer solution (pH less than 8) using a quinhydrone electrode.

14. To determine the pH of various mixtures of sodium acetate and acetic acid in aqueous solution and hence determine the dissociation constant of the acid.

15. Titrate potentiometrically Zn (II) by K4Fe(CN)6 and verify the composition of the complex K2Zn3 [Fe(CN)6]2

16. Determination of nitrite in water spectrophotometrically.

17. Determination of molecular weight of polymers by Turbidity metery.

18. Determine the molar refraction of a solid substance by dissolving it in a solvent and its refractive index.

MCH4113: NATURAL PRODUCTS IN CHEMISTRY

Credits : 05

LTP : 410

Course Description:

This course deal with biosynthetic pathways of natural products, terpenoids, steroids, alkaloids, haemin and chlorophyll, antibiotics, prostaglandins, peptides and proteins, carbohydrates and nucleic acid.

Course learning outcomes: After completion of this course, students will be able to:

CO1: to get knowledge about isoprene rule and terpenoids.

CO2: have idea about various synthesis methods of natural products.

CO3: to find structures and functions of different steroids.

CO4: to synthesize different type of alkaloids.

Course content:

Unit I

1. Studies on Biosynthetic Pathways of Natural Products

a) The acetate hypothesis, poly-ketoacids, their addol type cyclisations and meta orientations of hydroxyl groups in naturally occurring phenols. b) Isoprene rule, mechanism of formation of mevalonic acid from acetyl coenzyme, Biogenetic isoprene rule. Geranyl pyrophosphates and its conversion into alphapinene, thujene and borneol. Farnesyl pyrophosphate, geranyl, geranyl pyrophosphate and mechanistic considerations for their interconversions into cadinene and abietic acid.

Unit II

2. Terpenoids

General classification, general methods of structure determination, chemistry of camphor, abietic acid, santonin biosynthetic studies on tri and tetra terpenoids.

Unit III

3. Steroids

Occurrence, nomenclature and general methods of structure determination, isolation and general biosynthetic studies on steroids, chemistry of cholesterol, cortisone, progesterone, oestrone, transformations in steroid molecules.

Unit IV

4. Alkaloids

Definition, nomenclature and physiological action action occurrence, isolation and general methods of structure elucidation, and degradation, classification, chemistry of nicotine, quinine, papaverine, morphine and reserpine.

5. Porphyrins

Structure and synthesis of haemoglobin and chlorophyll.

Books Recommended:

1. Organic Chemistry by I.L. Finar Vol I & II

MCH4112: Chemistry of Materials

Credits : 05

LTP : 410

Course Description:

This course deals with solid state chemistry, macromolecules, glasses and ceramics and smart materials.

Course learning outcomes: After completion of this course, students will be able to:

CO1: learn about basic concepts of solid-state chemistry.

CO2: learn about synthesis methods of different types of polymers and determination of their molecular weight.

CO3: get knowledge about properties of glasses and ceramics.

CO4: learn properties and applications of super capacitors and nanomaterials.

Course content:

Unit I

1. Solid State Chemistry

Types of solids, band and bond theories, crystal lattice energy, point defects in metals and ionic compounds, energy and entropy of defects, their concentration, diffusion and electrical conduction via defects, non-stoichiometry types, colour centres and electrical properties of alkali halides, electron theories for metal conduction in metals and insulators, impurity semiconductors, reactions in organic solids, photochemical reactions, solid-solid reactions, decomposition and dehydration reaction.

Unit II

2. Macromolecules

Types of polymers, regular and irregular polymers, synthesis of polymers by chain and step reactions, physical properties of solid polymers (crystallinity, plasticity and elasticity), vulcanization of rubbers, molecular mass determination by osmometry, viscometry, light scattering and ultracentrifuge methods, number and mass average molecular masses, polymer solutions, factors affecting the solubility of polymers, conducting polymers, doping of polymers, mechanism of conduction, polarones and bipolarons.

Unit III

3. Glasses and Ceramics

Factors affecting glass formation, oxide glasses, electronegativity and bond type, viscosity, structural effects (zachariasen's rule (1932), criteria of SUN and Rawson, thermodynamics of glass formation, behavior of liquids on cooling, kinetics of crystallization and glass formation, structure of glasses: vitreous silica, silicate glasses, vitreous B2O3 and borate glasses, viscosiy, electrical conductivity of glasses and the mixed alkali effect, commercial silicate and borate glasses, metallic glasses, glass ceramics, refractories, important glass-ceramics compositions, properties of glass ceramics, applications.

Unit IV

4. Smart Materials

Methods of preparation-conventional ceramic methods, hot pressing and hot static pressing techniques, precursor method, gel method, co-precipitation method, glass crystallization methods, vacuum techniques- chemical vapor deposition method., organic superconductors, magnetism in organic materials, magnetic nano materials, energy storage materials, nanomaterials for targeted drug delivery, fullerenes as superconductors. High temperature ceramic superconductors, electrical and magnetic properties of superconductors, critical temperature Tc, thermodynamics of superconductors, London equation, BCS theory, applications.

Books Recommended:

1. Principles of polymer chemistry—P J Flory Cornell University Press
2. Physical chemistry of polymers—A J Tager, Mir Publishers
3. Physical chemistry of Macromolecules Tanford
4. Handbook of conducting polymers—T A Skotthem
5. Solid state physics—A J Dekker- Mac Millan Publishers
6. Solid state chemistry and its applications—A R West, Wiley Publishers
7. Solid state chemistry of drugs S R Byrn Academic Press
8. Chemistry of solid state—W.E. Garner Butterworth
9. Principles of physical chemistry—Puri-Sharma-Pathania, Vishal Publishers
10. Thermotropic Liquid crystals Ed. G W Gray John Wiley
11. Chemistry of polymers, Margarison and East
12. Polymer Chemistry, Malcolm, P, Stevens, Oxford University Press
13. Principles of Solid States, H. V. Keer, Wiley Eastern.

MCH4201: Advanced Organic Chemistry Laboratory

Credits: 02

LTP 002

Course Objectives:

This course deals with synthesis and reactivity of benzalacetophenone, synthesis of cyclohexene, preparation and characterization of aldol-dehydration, effects of substituents..

Course learning outcomes: After completion of this course, students will be able to:

CO1: get knowledge about chemical reactions involving benzal acetophenone.

CO2: learn about synthesis of cis and trans derivatives of cyclohexane diol**.**

CO3: prepare aldol condensation products.

CO4: get deep knowledge about substituent effect on aldehydes.

Course content:

1. Synthesis and Reactivity of benzal acetophenone

a. Bromination (Electrophilic additions) & subsequent debromination (Elimination)

b. Epoxidation (Cycloaddition, nucleophilic) and ring opening with hydroxide ion.

c. Michael addition of aniline.

d. Conversion of benzal acetophenone to its oxime (nucleophilic addition at C=O)

e. Conversion of oxime to amide (Beckmann rearrangement) and oxazole (Understand the reactivities at conjugated C=O and C=C) bond.

2. Synthesis of Cyclohexene from cyclohexanol and its conversion to 1, 2- cis and 1, 2- trans – cyclohexane diols.

a. Epoxidation with peracid (Cycloaddition) and anti- ring opening with sodium hydroxide to cis- cyclohexane -1, 2- diol.

b. Dihydroxylation with $KMnO_4$ (Mechanism of syn- and anti-cyclohexane-1, 2-diol)

3. Preparation and characterization of the aldol-dehydration products from various combinations of aromatic aldehydes and ketone.

4. Effect of substituents on aromatic aldehydes on the product distribution.

a. Aldehyde: benzaldehyde, 4-methylbenzaldehyde. 4-methoxy benzaldehyde.

b. Ketone: acetone, cyclopentanons, cyclohexanone.

Books recommended:

1. An Introduction to Modern Experimental Organic Chemistry, R.M. Roberts, J.C. Gilbert, L.B. Rodewald and A.S Wingrove, Holt Rinehart and Winston Inc, New York. 1969.

2. Vogel's Text Book of Practical Organic Chemistry.

3. Laboratory Experiments on Organic Chemistry, R. Edemas, J.R. Johnson and C.F. Wilcox, The Macmillan Limited, London, 1970.

4. Modern Projects and Experiments in Organic Chemistry, J.R. Mohrig, C.N. Hammonad, P.F. Schatz and T.C. Morrill, W.H. Freeman and Company, New York 2003.

MCH4202: Advanced Inorganic Synthesis Laboratory

Credits: 02

LTP 002

Course Description:

This course deal with synthesis of linkage isomers nitrito, synthesis of a coordination compound containing iron, synthesis of Ni(II) and separation of metal cations.

Course learning outcomes: After completion of this course, students will be able to:

CO1: synthesize cobalt complexes and perform their gravimetric analysis.

CO2: synthesize iron and nickel complexes and characterize them.

CO3: synthesize Schiff's base.

CO4: perform column and paper chromatography

Course content:

1. Synthesis of the Linkage Isomers nitrito- and nitropenta ammine cobalt (III) chloride

a) Preparation of chloropenta ammine cobalt (III) chloride, $[Co(NH_3)_5Cl]Cl_2$.

b) Preparation of nitropenta ammine cobalt (III) chloride, $[Co(NH_3)_5(NO_2)]Cl_2$.

c) Preparation of nitritopenta ammine cobalt (III) chloride, $[Co(NH_3)_5(ONO)]Cl_2$.

d) Estimate the chloride in all the complexes using gravimetric analysis.

e) Record and interpret the electronic absorption spectra and IR spectra of all cobalt (III) complexes and assign the observed change to distinguish the two isomers.

2. Synthesis of a coordination compound containing iron and analysis of this compound using redox methods

a) Preparation of iron (II) oxalate

b) Preparation of $K_3[Fe(C_2O_4)_3].3H_2O$

c) Characterization of Iron(II) and iron(III) complex with IR spectroscopy

d) Determination of iron and oxalate in $K_3[Fe(C_2O_4)_3].3H_2O$ using volumetric analysis

3. Synthesis and characterization of the Ni (II) complex of a Schiff-base ligand derived from Salicylaldehyde and ethylenediamine.

a) Synthesis the Schiff-base ligand.

b) Interpret the 1H NMR and IR spectra of the ligand.

c) Synthesis the Ni (II) complex of the ligand and compare its IR spectrum with that of the ons and use these to identify the cations present in the unknown mixtureligand.

4. Separation of the metal cations by

a) Column chromatography with gradient elution Co (II) and Ni (II). Analyze qualitatively the coloured fractions collected for separated cations.

b) Paper chromatography [Fe (II), Co (II), Ni (II) and Cu (II). Determine the Rf values for the separate standard cati.

Books recommended:

1. G. Marr, B. W. Rockett, Practical Inorganic Chemistry (1972).

2. *I. Grenthe, E. Nordin,* Inorganic Chemistry, *18 (1979) 1869–74.*

3. *J.C. Bailar, M. Eldon, Inorg. Synth. 1 (1939).*

MCH4203: Advanced Physical Chemistry Laboratory

Credits : 02

LTP 002

Course Description:

This course deal with chemical equilibrium, chemical kinetics, activity and activity coefficients, phase equilibrium, spectrophotometric methods, adsorption, turbidity metry and least square fitting.

Course learning outcomes: After completion of this course, students will be able to:

CO1: verify Debye Huckel Onsagar equation and study other equilibria.

CO2: study kinetics and mechanism of different reactions.

CO3: find activity coefficient and study phase diagrams.

Co4: learn about spectrophotometry, turbidity, adsorption isotherms and calibration methods.

Course content:

1. CHEMICAL EQUILIBRIUM

1. Study the effect of solvent on the conductance of AgNO3/acetic acid and determine the degree of dissociation and equilibrium constant in different solvents and their mixtures (DMSO, DMF, dioxane, acetone, and water) and test the validity of DEBYE HUCKEL-ONSAGER'S equation.

2. To determine acid and base dissociation constant of amino acid pH metrically.

3. To calculate thermodynamic parameters, G, S and H for the reaction,

Zn + Hg2SO4 = 2Hg + ZnSO4 by emf measurement.

2. CHEMICAL KINETICS

1. Study the salt effects and the solvent effect on the rate law of alkaline hydrolysis of crystal violet.

2. Determine the degree of hydrolysis and hydrolysis constant of CH3COONa/NaCl/aniline hydrochloride.

3. Determine the order of reaction by analysing the kinetic dependence of individual reactant (e.g. saponification of ester).

4. Determine the energy of activation for the reaction studied above.

5. Determine the relative rate of reaction of iodide ion with H_2O_2 at room temperature, using different concentrations of iodide ion (Clock reaction)

3. ACTIVITY AND ACTIVITY COEFFICIENTS

1. Determination of mean activity coefficient of given electrolyte by cryoscopy.

2. Determine activity coefficients by EMF method.

4. PHASE EQUILIBRIUM

1. Draw the phase diagram for any one of the following three component partially immiscible liquid systems.

I) DMSO/water/benzene ii) water/benzene/acetic acid.

5. SPECTROPHOTOMETRIC METHODS

1. To study the effect of extended conjugation on the wave length of maximum absorption of organic compounds.

2. Determine the dissociation constant of phenolphthalein calorimetrically.

3. Find the strength of CuSO4 solution by titrating it with EDTA spectrophotometrically.

6. ADSORPTION

1. To determine the adsorption isotherms of heavy metals like Cd, Zn, Cr, Pb, Ni by using non-conventional adsorbents.

7. TURBIDITY METRY

1. To determine concentration of sulphate ions with the help of turbidity meter.

2. Determine the CMC by turbidimetric method.

8. LEAST SQUARE FITTING

1. To draw calibration curve for the concentration determination of potassium ions by flame photometry and to study the least square fitting of the data.

Books recommended:

1. A. *Findlay,* Practical Physical Chemistry.

2. *J.B. Yadav,* Advanced Practical Physical Chemistry.

MCH3113: Ligand Field Theory

Credits : 05

LTP 410

Course Description:

This course deal with symmetry, molecular orbital theory for metal complexes, interelectronic repulsions, free ions in medium and strong crystal fields, magnetic properties and electronic spectra of transition metal complexes.

Course learning outcomes: Students will be able to:

CO1:Understand symmetry operations and MO theory applications.

CO2: learn about the point groups and symmetry operations of different molecules.

CO3: learn about electric and magnetic properties of complexes.

Co4: learn about racah parameters and energy level diagrams of complexes.

Unit I

1. Symmetry

Symmetry elements, symmetry operations and their matrix representation, group postulates and types, multiplication tables, point group determination, determination of reducible and irreducible representations, character tables, construction of character tables for C2v, C3v (non-abelian group), use of symmetry in obtaining symmetry of orbitals in molecules, use of character table to determine which metal orbitals are used in σ and π bond formation in octahedral, tetrahedral and square planar transition metal complexes, qualitative splitting of s, p, d, f orbitals in octahedral, tetrahedral and square planar fields using character tables and without the use of character tables.

SECTION -B

2. Molecular Orbital Theory for Metal Complexes

Recapitulations, ligands symmetry orbitals and metal orbitals involved in molecular orbitals formation in octahedral complexes, MOEL diagrams for octahedral tetrahedral and square planar complexes showing σ and π bonding in transition metal complexes.

3. Interelectronic Repulsions

Spin-spin, orbital-orbital and spin orbital coupling, LS and j-j coupling schemes, determination of all the spectroscopic terms of pn, dn ions, determination of the ground state terms for pn, dn, fn ions using L.S. scheme, determination of total degeneracy of terms, order of interelectronic repulsions and crystal field strength in various fields, two type of electron repulsion parameters, spin orbit coupling parameters (λ) energy separation between different j states, The effect of octahedral and tetrahedral fields on S, P, D and F terms (with help of the character table), splitting patterns of and G, H and I terms.

Unit III

4. Free Ions in Medium and Strong Crystal Fields

Strong field configurations, transition from weak to strong crystal fields, evaluation of strong crystal field terms of d2 configuration in octahedral and tetrahedral crystal fields (using group theory), construction of the correlation energy level diagrams of d2 configuration in octahedral field, study of energy level diagrams for higher configurations, selection rules of electronic transitions in transition metal complexes, their proof using group theory, relaxation of the selection rule in centrosymmetric and non-centrosymmetric molecules, Orgel diagrams, Tanabe-Sugano diagrams

5. Magnetic Properties

Van Vlecks formula for susceptibility, first order Zeeman effect, second order Zeeman effect, KT states, quenching of orbitals angular momentum by ligand field, the magnetic properties of A and E terms, the magnetic properties of T terms, electronic delocalization, magnetic properties of dn and fn metalions.

Unit IV

6. Electronic Spectra of Transition Metal Complexes

Variation of the Racah parameter, nephlauxetic effect-central field covalency, symmetry restricted covalency, differential radial expansion, spectrochemical series, band intensities, factors influencing band widths, discussion of electronic spectra of octahedral and tetrahedral d1– d9 metal ions, calculation of 10Dq and B with use of Orgel and Tanabe Sugano diagrams, low spin complexes of Mn3+, Mn2+, Fe3+, Co3+, Fe2+, comment on the spectra of second and third transition series, spectra of K3MoCl6 and [Rh(NH3)6]3+, spectra of cis and trans[Co(en)2X2]+, [Mn(H2O)6]2+, CuSO4.5H2O and its anhydrous complex, comparison of d–d band with f–f bands. Introduction to Charge Transfer Spectra.

Recommended Books:

1. F.A. Cotton, Chemical Application of Group Theory, Wiley Eastern.

2. G. L. Miessler, D. A. Tarr, Inorganic Chemistry, 3rd edition, Pearson Education.

3. B.N. Figgis, Introduction to Ligand Field, Wiley Eastern.

4. A.B.P. Lever, Inorganic Electronic Spectroscopy, Elsevier.

5. A. Earnshaw, Introduction to Magnetochemistry, Academic Press.

6. J.E. Huheey, Inorganic Chemistry Principles of Structure and Reactivity, Harper.

7. R.S. Drago, Physical Method in Chemistry, W.B. Saunders Company.

8. F.A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, Wiley.

MCH3125: SPECTROSCOPY–A: Techniques in Structure Elucidation of Organic Compounds

Credits : 05

LTP : 410

Course Description:

This course deals with nuclear magnetic resonance, mass spectroscopy, ultraviolet and visible spectroscopy, infrared spectroscopy, applications in organic chemistry and solution of structural problems.

Course learning outcomes: Students will be able to:

CO1: learn basics of NMR, IR, UV spectroscopy and mass spectrometry.

CO2: get knowledge about applications of various spectroscopic techniques.

CO3: learn to interpret the unknown materials after completing this course.

CO4: will enhance the ability of students to solve the combined problems on the different spectroscopic techniques.

Course content:

Unit I

1. Nuclear Magnetic Resonance

The Nuclear spin, Larmor frequency, the NMR isotopes, population of nuclear spin level, spin and spin lattice relaxation. Measurement techniques (CW & FT method), solvent used. Chemical shift, reference compounds, shielding constant, range of typical chemical Shifts simple application of chemical shifts, ring current and aromaticity. Shifts for H and 13C - Spin-spin interactions, low- and high-resolution spectra with various examples, Correlation of H bound to carbon, H bound to other nuclei such as nitrogen, oxygen, sulphur, complex spin-spin interaction between two or more nuclei.

Effect of chemical exchange, fluxional molecules, Hindered rotation on NMR spectrum Karplus

relationship, nuclear magnetic double resonance, chemically induced dynamic nuclear polarization. Brief introduction to multipulse NMR spectroscopy, Application of structure elucidation of simple organic molecules lanthanide shift.

Unit II

2. Mass Spectroscopy

Elementary theory - measurement techniques (EI, CI, FD, FAB), resolution, exact masses of nuclides, molecular ions, isotope ions, fragment ions of odd and even electron types, rearrangements, factors affecting cleavage patterns, simple cleavage, cleavages at a hetero atom, multicentre fragmentations rearrangements, Retro Diels–Alder fragmentation. Cleavage associated with common functional groups (aldehydes, ketones cyclic and acyclic esters, alcohols, olefins, aromatic compounds amines). - Special methods of GCMS, high resolution MS, Introduction to radical anion mass spectroscopy. Interpretation of the spectrum of an unknown.

Unit III

3. Ultraviolet and Visible Spectroscopy

The energy of electronic excitation, measurement techniques, Beer-Lambert law, molar extinction coefficient. The Frank Condon principle. Different types of transition noticed in UV-Vis spectrum of organic functional groups and their relative energies. Chromophore, auxochromes, factors affecting absorption max, effect of steric hindrance to coplanarity, solvent effects. Applications of UV-Vis spectroscopy.

4. Infrared Spectroscopy

Vibrational energy levels, selection rules, force constant, fundamental vibration frequencies, factors influencing vibrational frequencies (vibrational coupling, hydrogen bonding, electronic effect, bond angles, field effect). Sampling techniques, absorption of common functional groups, interpretation, finger print regions.

Applications in Organic Chemistry

a. Determining purity and quantitative analysis.
b. Studying reaction kinetics.
c. Determining purity and quantitative analysis.
d. Studying hydrogen bonding.
e. Studying molecular geometry & conformational analysis.
f. Studying reactive species

Books Recommended:

1. W. Kemp. Organic Spectroscopy.
2. W. Kemp. N.M.R. Spectroscopy.
3. D.H. Williams and I. Fleming. Spectroscopic Methods in Organic Chemistry.
4. R.M. Silverstein & G.C. Bassler, Spectrometric Identification of Organic Compounds.
5. R.C. Banks, E.R. Matjeha and G. Mercer, Introductory Problems in Spectroscopy.
6. Introduction to Spectroscopy – Pavia

MCH3112: REACTION MECHANISMS AND METAL CLUSTERS

Credits : 05

LTP : 410

Course Description:

This course deal with reaction mechanism of transition metal complexes, electron transfer process, doubly bridged inner sphere transfer, metal ligand equilibria in solution and inorganic rings, chains and metal cluster.

Course learning outcomes: Students will be able to:

CO1: get knowledge about chemical reactions of transition metal complexes.

CO2: learn about electron transfer processes, stability of complexes and structures of inorganic compounds.

CO3: learn about metal-liquid equilibrium.

CO4: learn about the heterocyclic inorganic rings in detail.

Course content:

Unit I

Reaction Mechanism of Transition Metal Complexes

Inert and labile complexes, mechanisms of substitution (dissociative, associative interchange mechanism, the conjugate mechanism, substitution in trans complexes, substitution in cis complexes, isomerism of chelate rings), trans effect, explanation for trans effect, ligand substitution reactions of square planar and octahedral complexes: their factors and mechanism of substitution, orbital occupation mechanisms. Anation reaction, Metal carbonyl reactions species with 17 electrons.

Unit II

Electron transfer processes with mechanism, key ideas concerning electron transfer reactions between transition Metals. Cross reactions and thermodynamics. Marcus theory, its kinetics and applications.

Unit III

Doubly bridged inner sphere transfer and other electron transfer reactions. Two electron transfer, non-complementary reactions. Stereochemical nonrigidity of coordinate and organometallic compounds, trigonal bipyramid, system with six or more coordination number.

Isomerization and racemization of trischelates, metal carbonyl scrambling.

Metal-ligand Equilibria in Solution

Stepwise and overall formation constant and their interaction, trends in step wise constant, factors affecting the stability of metal complex with reference to the nature of metal ion and ligand chelate effect and its thermodynamic origin. Determination of binary formation constants by pH-meter, Job's method and spectrophotometry.

Unit IV

Inorganic Rings, Chains and Metal Cluster

Borazines, Phosphazenes and other heterocyclic inorganic ring systems, homocyclic in organic systems, cages of P and S, oxides & sulphides, higher boranes and carboranes, methods of classifying boranes, molecular orbit view of chlorohydroborane ions and carboranes metallocarboranes, isopoly and heteropoly acids and salts; metal-metal bonds and bi-, tri-, tetra-, penta-, and hexa-nuclear clusters, electron counting schemes for HNCC's. Approaches to systematic cluster synthesis; mention of seven, eight and nine atom clusters. Isolobal analogy and examples of application of analogy.

Books Recommended:

1. K.P. Purcell and J. V. Kotz: Inorganic Chemistry W.B. Saunders Co. London, (1977).
2. G. L. Miessler, D. A. Tarr, Inorganic Chemistry, 3rd edition, Pearson Education.
3. F.A. Cotton & Wilkinson: Inorganic Chemistry V & VI Ed. Willy Eastern – (1999).
4. J.E. Huheey: Inorganic Chemistry III & IV Ed. Pearson Education Asia.

MCH3111: SPECTROSCOPY – B:

Techniques for Structure Elucidation of Inorganic Compounds

Credits : 05

LTP : 410

Course Description:

This course deal with vibration and rotation spectroscopy, symmetry and point groups, photo electron spectroscopy, electron spin resonance spectroscopy, nuclear quadrupole resonance spectroscopy and Mossbauer spectroscopy.

Course learning outcomes: Students will be able to:

CO1: learn basics of vibrational and rotational spectroscopy.

CO2: learn symmetry operations and how to find point groups.

CO3: acquire basic knowledge about PES, ESR, NQR and Mossbauer spectroscopies.

CO4: students will be able to interpret the structure of synthesized inorganic materials after completing this course.

Course content:

Unit I

Vibration and Rotation Spectroscopy: Infrared, Raman and Microwave (Book 2)

Harmonic and Anharmonic oscillators, vibrational energies of diatomic molecules. Potential energy function for a chemical bond. Absorption of radiations by molecular vibration. Selection rules, force constant.

Rotational energies of linear molecules. Rotational energy level populations, merits and demerits of microwave spectroscopy, rotational spectra of rigid, linear molecules, non-rigid rotators. Determination of moment of inertia and bond length from rotational spectra, relative intensities of spectral lines. Rotational spectra of non-linear molecules (brief mention), vibrations in polyatomic molecules. Effects giving rise to absorption bonds. Group vibrations and limitations of group vibration concepts. Polarizations of light. Theories of Raman effect, merits and demerits of Raman spectroscopy. Pure rotational Raman spectra of linear molecules. Vibrational Raman spectra selection rules. Rule of mutual exclusion. Rotational fine IR spectra, vibronic coupling. Sample handling. Factors affecting absorption frequencies, interpretation and finger printing regions.

Unit II

Symmetry and Point Groups: (Book 2)

Definition of symmetry, symmetry elements, determination of point groups, introduction to use of character table in determining irreducible representation and symmetry of the atomic orbitals.

Use of symmetry considerations to determine the number of active I.R, and Raman lines (character tables to be provided in the Examination).

Applications of Raman and IR selection rules to the determination of Inorganic structure with special emphasis on:

I. Metal carbonyls.

ii. NSF3

iii. Geometrical isomerism – differentiation between cis and trans [Co(bipy)2Cl2]Cl.

iv. Structures of CO_2, N_2O, H_2O, chloro complexes of mercury, cadmium and zinc and some octahedral complexes ML6 (e.g., SiF62-, PF5-, SF6).

v. Changes in the spectra of donor molecules upon coordination with special emphasis on N, N–dimethylacetamide and DMSO with Fe3+, Cr3+, Zu2+, Pd2+ and Pt2+ ions. IR spectroscopy and modes of coordination of SO42-, N_2, O_2, NO, CO_{32} - , NO_3.

Unit III

Photo Electron Spectroscopy (Book 1, 2 and 3)

Introduction, excitation & ejection of electrons, electronic energy levels in atoms and molecules, Core level photoelectron spectroscopy, symmetry & molecular orbitals, valence electron photoelectron spectroscopy, valence excitation spectroscopy. Dissociation, Predissociation, change of shape on excitation.

Electron Spin Resonance Spectroscopy (Book 1, 2, 3 and 5)

Features of ESR spectra, measurement technique hyperfine coupling in isotropic system (C5H5, C6H6, C14H10, biphenyl), anisotropic splitting, electron–electron interaction, transition metal complexes g-value and factors affecting g-value, zero field splitting, Kramer's degeneracy, rate of electron exchange, application to p–benzosemiquinone, DPPH, pyrazine. Double resonance technique ENDOR, ELDOR.

Unit IV

Nuclear Quadrupole Resonance Spectroscopy (Book 2)

Introduction, effects of magnetic field on the spectra. Relationship between the electric field gradient and molecular structure. Interpretation of eQ, data, the effect of crystal lattice on the magnitude of eQ4, double resonance technique, Application (PFCI4.PCI5), (NH4)2TeCl6, group 14 tetra halides, R3MX2 (M=As, Sb, Bi), cis & trans [Co(en)2Cl2]Cl, polyhalide ion, BrCN, HIO3.

Mossbauer Spectroscopy (Book 1,2,4,6)

Introduction, principles, conditions of MB spectra, parameters from MB spectra. Isomer shift electric quadrupole interaction, magnetic interaction, use of additive partial quadrupole splitting to predict quadrupole coupling. Application of {57Fe, 119Sn, 151Eu compounds, to biological systems to surface study, I2CI6, IBr2 CL4, XeF4, XeCI4.

Books Recommended:

1. E.A.V Ebsworth; W.H Renkin; Cradock, Structure Methods in Inorganic Chemistry.
2. R.S Drago, Physical Methods for Chemists (Ist and IInd Edition).
3. C.N Banwell, Fundamentals of Molecular Spectroscopy.
4. S. Walker and H. Straughan Spectroscopy, Vol. I.
5. J.E. Wertz & J.R. Bolton, Electron Spin Resonance (p.49-65).
6. N.N. Greenwood & T.C Tibb, Mossbauer Spectroscopy.
7. K. Nakamoto, Infrared Spectra of Inorganic and co-ordination Compounds.

MCH3116: Electrochemistry and Chemical Dynamics

Credits : 05

LTP : 410

Course Description:

This course deals with electrochemistry, chemical dynamics, voltammetry and polarography.

Course learning outcomes: Students will be able to:

CO1: learn about Debye equations and other theories related to electrochemistry.

CO2: get knowledge about rate law expressions.

CO3: learn about different theories in chemical dynamics.

CO4: learn about basics of voltammetry and polarography.

Course content:

Unit I

Electrochemistry

Electrochemistry of solutions, Debye-Huckel-Onsager treatment and its extension, ion-solvent interactions, Debye-Huckel-Bjerrum mode, Thermodynamics of electrified interface equation, Derivation of electro-capillarity, Lipmann equation (surface excess), method of determination, structure of electrified interfaces, Guoy-Chapmann, Stern models, overpotential, exchange current density, derivation of Butler-Volmer equation, Tafel plot. Semiconductor interface theory of double layer at semiconductor electrolyte solution interface, structure of double layer interfaces, effect of light at semiconductor solution interface. Introduction to corrosion, homogeneous theory, forms of corrosion, corrosion monitoring and prevention

Unit II

Chemical Dynamics

Methods of determining rate laws, collision theory of reaction rates, steric factor, activated complex theory, Arrhenius theory and activated complex theory, ionic reactions, kinetic salt effects, treatment of unimolecular reactions, Lindemann-Hinshelwood theory.

Unit III

Chemical Dynamics

Dynamic chain (hydrogen bromine reaction, pyrolysis of acetaldehyde, decomposition of ethane), photochemical reactions between hydrogen-bromine and hydrogen-chlorine, oscillatory reactions (Belousov-Zhabotinsky reactions), homogeneous catalysis and kinetics of enzyme reactions, general features of fast reactions, study of fast reactions by flow method, relaxation method, flash photolysis, nuclear resonance.

Unit IV

Voltammetry and Polarography

Polarography, polarographic cells, polarogram, interpretation of polarographic waves, equation for the polarographic waves, effect of complex formation on polarographic wave, polarograms for irreversible reactions, dropping mercury electrode (DME), current variations during life time of a drop, merits and demerits of DME, polarographic diffusion currents, Ilkovic equation, capillary characteristics, temperature, polarograms for mixture of reactants, anodic and cathodic waves, factors affecting polarographic currents, applications of polarography, treatment of data, organic and inorganic polarographic analysis, voltammetry at solid electrodes, cyclic voltammetry and interpretation of data, pilot-ion and standard addition method for quantitative analysis.

Books Recommended:

1. Chemical Kinetics, K. J. Laddler, McGraw-Hill
2. Modern Electrochemistry Vol.1,2,3, J. Bochris and A.K.N. Reddy
3. Fundamentals of electrochemistry; P. Monk
4. Principles of Instrumental Analysis; Skoog, West; Saundres Publications

MCH3117: PHOTOCHEMISTRY AND PERICYCLIC REACTIONS

Credits : 05

LTP : 410

Course Description:

This course deals with molecular orbital symmetry, cycloaddition reactions, electrocyclic reactions, sigma tropic rearrangements, photochemical reactions, determination of reaction mechanism, photochemistry of alkenes, photochemistry of carbonyl compounds, photochemistry of aromatic compounds and miscellaneous photochemical reactions..

Course learning outcomes: Students will be able to:

CO1: get idea about frontier orbitals and perturbation theory.

CO2: learn about different reactions involving pericyclic reactions.

CO3: learn about photochemical reactions and their mechanism.

CO4: learn about photochemistry of vision.

Course content:

Unit I

Pericyclic Reactions

(1) Molecular Orbital Symmetry

Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene, allyl system, classification of Pericyclic reactions FMO approach. Woodward-Hoffmann correlation diagrams method and Perturbation of molecular orbital (PMC) approach for the explanation of pericyclic reactions under thermal and photo-chemical conditions.

(2) Cycloaddition Reactions

Antrafacial and suprafacial additions, notation of cycloadditions (4n) and (4n+2) systems with a greater emphasis on (2+2) and (4+2) cycloaddition-stereochemical effects and effects of substituents on the rates of cycloadditions, 1,3-dipolar cyclo-additions and cheleotropic reactions.

Unit II

(3) Pericyclic Reactions: Electrocyclic reactions

Controtatory and disrotatory motions, 4n, 4n+2, allyl systems, secondary effects.

(4) Sigmatropic Rearrangements

Suprafacial and antrafacial shifts [1,2]- sigmatropic shifts involving carbon moieties retention and inversion of configuration, [3,3] and [5,5] sigma-tropic rearrangements, detailed treatment of Claisen and Cope rearrangements, fluxional tautomerism, Aza-Cope rearrangements, introductions to Ene reaction, simple problems on pericyclic reactions. Electrocyclic rearrangement of cyclobutenes and 1, 3-cyclohexadienes.

Unit III

Photochemistry

(5) Photochemical Reactions

Interaction of electromagnetic radiation with matter, types of excitations, fate of excited molecule, quantum yield, transfer of excitation energy, actinometry.

(6) Determination of Reaction Mechanism

Classification, rate constants and life times of reactive energy states–determination of rate constants of reactions. Effect of light intensity on the rate of photochemical reactions. Types of photochemical reactions–photodissociation, gas-phase photolysis.

Unit IV

(8) Photochemistry of Carbonyl Compounds

Intramolecular reactions of carbonyl compounds – saturated, cyclic and acyclic, β, γ-unsaturated and α, β-unsaturated compounds, Cyclohexadienones. Intermolecular cycloaddition reactions –dimerization and oxetane formation.

(9) Photochemistry of Aromatic Compounds

Isomerizations, additions and substitutions.

(10) Miscellaneous Photochemical Reactions

Photo-Fries reactions of anilides. Photo-Fries rearrangement. Barton reaction. Singlet molecular oxygen reactions. Photochemical formation of smog. Photodegradation of polymers. Photochemistry of vision.

Books Recommended:

1. Organic Photochemistry – Chapman and Depuy.
2. Organic Photochemistry – W.H. Horsepool.
3. Photochemistry of Excited States – J.D. Goyle.

MCH3114: MATHEMATICS FOR CHEMISTS

Credits : 05

LTP : 410

Course Description:

This course deals with basic of mathematics.

Course learning outcomes: Students will be able to:

CO1: handle calculations related to trigonometry, matrices and determinants..

CO2: handle calculations related to matrices and determinants.

CO3: find out results of differentiation.

CO4: find out results of integration.

Course content:

Unit I

Trigonometry and Determinants:

Definition of sin, cos, tan, cot, sec, cosec functions with the help of unit circle, values of sin x, cos x for x = 0, /6, /3, /2. Trigonometric identities (without proofs) and their applications.

Definition and expansion properties of determinants, product of two determinants of 3rd order.

Unit II

Matrices:

Introduction to various forms of Matrices, row, column, diagonal unit, Sub matrix, square, equal matrices, null, symmetric and skew symmetric matrices, transpose of a matrix, adjoint and inverse of matrices. Addition, multiplication, characteristic equation of a matrix, statement of Cayley Hamilton theorem. Rank of matrix, condition of consistency of a system of linear equations. Eigen vectors and Eigen values of matrices.

Unit III

Differential Calculus

Differentiation of standard functions, theorems relating to the derivative of the sum, difference, product and quotient of functions (without proofs), derivative of trigonometric functions, inverse trigonometric functions, logarithmic functions and exponential functions, differentiation of implicit functions, logarithmic differentiation.

Unit IV

Integral Calculus

Integration as an inverse of differentiation, summation, area under a curve, indefinite integrals of standard forms, method of substitution, method of partial fractions, integration by parts, definite integrals, reduction formulae, definite integrals as limit of a sum and geometrical interpretation.

Books Recommended:

1. Santi Narayan & P.K. Mittal – Differential Calculus.
2. Santi Narayan & P.K. Mittal - Integral Calculus.
3. B.S. Grewal – Higher Engineering Mathematics.
4. Joseph B. Dence – Mathematical Techniques in Chemistry.
5. Margenau and Murphy, the Mathematics of Physics and Chemistry.
6. B.L. Moncha and H.R. Choudhary – A Text Book of Engineering Mathematics

MCH3115: BIOLOGY FOR CHEMISTS

Credits : 05

LTP : 410

Course Description:

This course deals with basics of biology.

Course learning outcomes: Students will be able to:

CO1: learn about biomolecules, cell organelles and genetics.

CO2: learn about diverse form of living beings.

CO3: learn about structure of DNA and RNA.

Co4: learn about structure of viruses.

Course content:

Unit I

The Organisation of Life

1. Biologically important molecules: Carbohydrates, lipids, proteins and nucleic acids.
2. The life of cells – The cell theory, general characteristics of cells, difference between prokaryotic and eukaryotic cells, difference between plant and animal cells, cell organelles.

Unit II

3. Tissues, organs and organ systems: Animal tissues; epithelial tissues, connective tissues, muscle tissue, nervous tissue and neoplasia; plant tissue: meristematic tissue, permanent tissues.

Unit III

Genetics

1. The basic principle of heredity: Mendel's law, monohybrid cross, dihybrid cross.
2. DNA – Double helix structure and replication.
3. Genes expression: Transcription and translation, genetic code.

Unit IV

The Diversity of Life

1. The classification of living things – criteria of classification, Whittaker's systems of classification, their characteristics with are example of each.
2. Viruses, structure of viruses.

Unit IV

The Diversity of Life

1. The classification of living things – criteria of classification, Whittaker's systems of classification, their characteristics with are example of each.
2. Viruses, structure of viruses.

Books Recommended:

1. Cord Biology - South Western Educational Publications, Texas, 2000.

MCH3118: MEDICINAL CHEMISTRY

Credits : 05

LTP : 410

Course Description:

The aim and objective of this course is to familiarize students with the basic concept of medicinal chemistry. Emphasis will be made on the SAR of various drugs such as antimicrobial, antifungal and their mode of actions. The commercial synthesis of representative of such drugs will also be discussed.

Course learning outcomes: Students will be able to:

CO1: Understand the need of Medicinal Chemistry in curing various ailments.

CO2: Study the concept of antimicrobial and anti-protozoal drugs.

CO3: Study the SAR of antimicrobial and anti-protozoal drugs.

CO4: Understand the total synthesis of antimicrobial and anti-protozoal drugs.

Course content:

Unit I

Antibacterial Drugs: Structure, stereochemistry, mode of action, structure activity relationships (SAR), specific clinical applications of following classes of pharmaceuticals with synthetic/commercial route to the indicated examples. Penicillin, cephalosporins, tetracyclines, aminoglycosides, chloramphenicol, macrolides, lincomycins, polypeptides antibiotics, polyene antibiotics. Sulfonamides and sulfones fluoroquinolines, trimethoprim and other unclassified antibiotics. Antimycobacterial: Sulfanilamide's, p-aminosalicyclic acid derivatives, thioamides, thiourea derivatives, thiosemicarbazones, isoniazid, kanamycin sulfate, capreomycin, rifampin, pyrazinamide, ethionamide, clofazimine, cyclosporin, dapsone, sulfazem. Commercial synthetic/semi-synthetic routes to: 6-aminopenicillanic acid, ampicillin, amoxycillin, production of penicillin, 7-aminocephalsporanic acid, cephalexin, ceftizoxime, cefaclor, cephalothin, tetracyclines: doxycycline, nalidixic acid, sulfadiazine, norfloxacin, ciprofloxacin, O-ofloxacin, amifloxacin, difloxacin, chloramphenicol, nitrofurantoin, sulfamethoxazole, acetylsulfisoxazole, trimethoprim.

Unit II

Antiamoebic and antiprotozoal drugs: emetine hydrochloride, 8-hydroxyquinoline, iodochlorhydroxyquin, metronidazole, diloxanidefuroate, bilamical hydrochloride, hydroxy stilbamidineisothinate, pentamidine isothionate, nifurtimox, suramin sodium, carbarsone, glycobiarsol, melarsoprol, sodium stibogluconate, dimercaprool, diethylcabamazine citrate, centarsone, acetarsone, antimony potassium tartrate, bismuth sodium thioglycollate, sulphonamide, stibiophen, bismuth sodium thioglycollamate, furazolidone. Commercial synthetic routes to: metronidozole, ronidazole, flunidazole, iodoquinol, nifurfimax, benzindazole, tryparsamide.

Unit III

a. Antimalarial Drugs: cinchona alkaloids, 4-aminoquinolines, 8-aminoquinolines, 9-aminoacridines, biguanides, pyramidines and sulfones, mefloquine, sulfonamides. Commercial synthetic routes to: chloroquine, pamaquine, primaquine, proguanil, amodiaquine, mefloquine, pyremethamine, pontoquine.

b. Anthelmintic Drugs: Introduction, tetrachloroethylene, piperazines, gentian violet, pyrviniumpamoate, thiabendazole, mabendazole, bephenium hydroxynaphthoate, dichlophene, niclosamide, levamisole hydrochloride, tetramisole, niridazole, biothional, antimony potassium tartarate, stibiophen, sodium stibiocaptate.

Unit IV

Antifungal Drugs: Fatty acids and their derivatives (propionic acid, zinc propionate, sodium caprylate, zinc caprylate, undecylenic acid, zinc undecylenate, triacetin), salicylanilids, salicyclic acid, tolnaftate, p-chloromethoxylenol, acrisocrin, fluconazole, itraconazole, haloprogin, clotrimazole, econazole, miconazole, ketoconazole, flucytosine, griseofulvin, polyene antibiotics (nystatin, amphoetericin-B), chlorophenesin, dithranol. Commercial synthetic routes to: miconazole, clotrimazole, econoazole, fluconazole, griseofulvin, ketoconazole, nafttidine, tolnaftate, flucytosin.

REFERENCES & TEXT BOOKS:

1. W.O. Foye, T.L. Lamke, D.A. Williams, Principles of Medicinal Chemistry, 5th Edition, Lippencott Williams and Wilkins, 2002

2. B.G. Reuben and H.A. Wittcoff; Pharmaceutical Chemicals in Perspective; John Wiley & Sons, New York, 1989.

3. R.F. Deorge; Wilson and Gisvolds Textbook of Organic Medicinal and Pharmaceuticals Chemistry, 8th ed.; J.B. Lippincott Company, Philadelphia, 1982.

MCH3119: ADVANCED FUNCTIONAL MATERIALS

Credits : 05

LTP : 410

Course Description:

To introduce the students in the area of various functionalized materials, their synthesis and their properties with emphasis to their applications.

Course learning outcomes: Students will be able to:

CO1: understand the basic concepts and formation of various carbon nano tubes and its functionalization.

CO2: know the types and structure of functionalized fullerenes.

CO3: learn the common and important synthesis methods, structure and composition of organic polymers and its properties and applications.

CO4: understand the synthesis and applications of antimicrobial biopolymers, learn the various approaches for the synthesis of nanoscale materials/nanoparticles and their properties and applications.

Course content:

Unit I

3-D Carbon-rich p-systems – nanotubes and segments: functionalization of carbon nanotubes, introduction to carbon nanotubes – a new carbon allotrope, functionalization of carbon nanotubes, covalent functionalization, halogenation of carbon nanotubes, fluorination of carbon nanotubes, chlorination of carbon nanotubes, bromination of MWCNTs, chemical derivatization of "Fluoronanotubes", oxidation of CNTs – oxidative purification, carboxylation of CNTs, defect functionalization–transformation of carboxylic functions, hydrogenation of carbon nanotubes, Addition of radicals, addition of nucleophilic carbenes, sidewall functionalization through electrophilic addition, functionalization through cycloadditions, addition of carbenes, addition of nitrenes

Unit II

Cyclophenacene cut out of fullerene: - introduction, synthesis of [10] cyclophenacene β-conjugated systems from [60] fullerene, synthetic strategy, synthesis and characterization of [10] cyclophenacenes, structural studies and aromaticity of [10] cyclophenacene, synthesis

of dibenzo-fused corannulenes. Strategic advances in chromophore and materials synthesis introduction, oligomers with a tetrahedral core unit, oligomers with a tetrasubstituted benzene core, oligomers with a tetrasubstituted biaryl core.

Unit III

Advanced biodegradable organic polymers: introduction, synthesis of biodegradable polymers by polycondensation, general polycondensation technique, post polycondensation technique, chain-extension technique, enzyme-catalyzed polycondensation, synthesis of biodegradable polymers by ring-opening polymerization, monomers, polymerization with metal catalysts, polymerization using metal-free organic catalystse.

Unit IV

Antimicrobial Biopolymers: introduction, biopolymers, ε-poly-l lysine, chitin and chitosan, synthetic biodegradable polymers, quaternary polymers, polyethylenimine, antimicrobial peptide mimics, metal loading, silver, magnesium, zinc, titanium, assessment of antimicrobial/antifungal testing methods.

Reference & Text Books:

1. Thomas J.J. Müller, Uwe H.F. Bunz , Functional Organic Materials Volume-I, Wiley-VCH

2. Hee-Gweon Woo , Hong Li; Advanced Functional Material; Springer

MCH3120: GREEN CHEMISTRY

Credits : 05

LTP : 410

Course Description:

To introduce the students about various concepts of green chemistry and its technologies. The emphasis is on the synthesis of various entities using benign methods of green chemistry.

Course learning outcomes: Students will be able to:

CO1: Conceptualize the various syntheses using novel and greener methods.

CO2: Predict the relationships between organic chemical structures and their reactivity in different greener and benign conditions.

CO3: Learn the fundamental and advanced concepts of green chemistry in reaction mechanisms.

CO4: Apply the new methodologies for altering the reactivity patterns of substrates and synthesize various molecules using combinations of reactive species in novel conditions.

Course content:

Unit I

Introduction to the green chemistry, historical context: the greening of chemistry; waste production, problems, prevention; measuring and controlling environmental performance; planning for the future for reducing carbon in the atmosphere, emergence of green chemistry and its environmental impact.

Unit II

Twelve principles of green chemistry, concepts, importance and their applications with special emphasis on the use of alternative renewable feedstock (bio-fuels, biomass and their applications in green synthesis of various compounds), use of innocuous reagents in natural processes, alternative solvents, design of the safer chemicals, designing alternative reaction methodology, minimizing energy consumption. Sustainable polymers: the case of polylactide, using CO2 and other feedstock.

Unit III

Green reactions (role, advantages and applications): aqueous phase organic synthesis, solvent less organic synthesis, photochemical organic synthesis, PTC catalyzed reactions, microwave induced reactions, enzymatic transformations, sonication reactions & reactions in ionic liquids

Unit IV

Green reactions (role & mechanism): Aldol condensation reaction (solid phase and ionic liquid synthesis), Baeyer-Villiger oxidation (aqueous phase and solid phase synthesis), Baylis-Hillman Reaction (microwave synthesis and ionic liquid synthesis), Biginelli reaction under microwave irradiation, Cannizaro reaction under sonication, Dakin reaction under ultrasonication, Darzen reaction in PTC, Dieckmann condensation (polymer supported synthesis), Diels-Alder reaction (in water, ionic liquid, MW and sonication), Photo Fries rearrangement, Stille coupling in water and SC-CO2, Ullmann reaction under sonication and in aqueous medium, Sonogashira reaction.

Reference & Text Books:

1. Anastas, P. T.; Warner, J. C. Green Chemistry: Theory and Practice; Oxford University Press: New York, 1998.

2. Lancaster, M.; Green Chemistry an Introductory Text; Royal Society of Chemistry, Cambridge, UK 2002.

MCH3121: SUPRAMOLECULAR CHEMISTRY

Credits : 05

LTP : 410

Course Description: To impart in depth knowledge of non-covalent interactions in supramolecular systems and their applications.

Course learning outcomes: Students will be able to:

CO1: To learn the fundamental concepts of supramolecular chemistry such as Host guest chemistry/ self-assembly.

CO2: Various kinds of non-covalent interactions occurring in supramolecular systems. .

CO3: Molecular recognition and nature of bindings involved in biological systems.

CO4: Structure of supramolecules of various types in solution and solid state and applications of supramolecules in miniaturization of molecular devices.

Course content:

Unit I

Host-Guest Chemistry: definition-supramolecular chemistry, host-guest and self-assembly; selectivity, preorganization and complementarity of binding sites, chelate ring size effect, donor group and orientation; binding constants, thermodynamic and kinetic selectivity; solvent effects and non- covalent interactions.

Unit II

Solution host-guest chemistry and ion recognition: macrocyclic acyclic hosts, templates effect and high dilution synthesis; cation recognition: crown ethers, lariat ethers, podands, cryptands, spherands, calixarenes, siderophore, inclusion compounds, molecular clefts and tweezers; anion recognition: challenge in anion receptor chemistry, charged and neutral receptors, contact ion pairs, cascade complex, remote anion and cation binding sites.

Unit III

Basic concepts of self-assembly and classification: self-assembly in synthetic systems: template effects in synthesis, self-assembly with covalent modification, a thermodynamic model: self-assembly of zinc porphyrin complexes, cooperativity and the extended site binding model self-assembly in biological systems: biological self-assembled fibers and layers, amyloids, actins and fibrin, bacterial s-layers, single molecule self-assembly: proteins and foldamers, strict self-assembly: the tobacco mosaic virus and DNA.

Unit IV

Catenanes and rotaxanes: statistical approaches to catenanes and rotaxanes, π–π and hydrogen bonded rotaxanes and catenanes, metal and auxiliary linkage approaches to catenanes and rotaxanes. Molecular devices, logic gate, molecular switches, molecular motor.

Reference & Text Books:

1. J. W. steed, J. L. Atwood; Supramolecular Chemistry, Second edition; 2009, Wiley

2. Jean-Marie Lehn; Supramolecular Chemistry; 1995, Wiley

3. K. Ariga, T. Kunitake; Supramolecular chemistry fundamental and applications; 2006, Springer

MCH3124: BIO-INORGANIC CHEMISTRY

Credits : 05

LTP : 410

Course Description: This course deals with metal ions, transport and storage of dioxygen, electron transfer, bioenergetics and ATP cycle, bio redox agents and mechanism.

Course learning outcomes: Students will be able to:

CO1: know the importance of metal ions in biochemistry.

CO2: have knowledge about dioxygen and electron carriers, enzymes and coenzymes.

CO3: learn about the importance of different metal and non-metals in human body.

CO4: learn about the role of enzymes in living systems.

Course content:

Unit I

1. Metal Ions in Biological Systems- Essential and trace elements, periodic survey of essential and trace elements, biological importance and relative abundance, Na+/ K+ ion pump.

2. Biochemistry of Iron- Availability of iron, competition for iron, iron toxicity and nutrition.

3. Metal Storage, Transport- Ferritin, transferrin and siderophores.

4. Metals in Medicine-Metal deficiency and disease, toxic effects of antibiotics and related compounds, chelate therapy.

Unit II

5. Transport and Storage of Dioxygen- Oxygen carriers-Hb and Mb: structure and mechanism of their function, cooperativity, inhibition and poisoning by ligands and metal ions, hemocyanins and hemerythrin, model complexes of iron, cobalt and copper.

6. Electron Transfer in Biology- Cytochromes-structure and function, CN- and CO poisoning, Ferredoxin and rubredoxin.

Unit III

7. Bioenergetics and ATP Cycle- Process concept to phosphate hydrolysis, nucleotide transfer-DNA polymerase, phosphate transfer pyruvate kinase, phosphoglucomutase, creatine kinase, ATPase. Photosynthesis and respiration – chlorophyll: structure, function and its synthetic model.

8. Nitrogenase- Biological N2 fixation, molybdenum nitrogenase, spectroscopic and other evidence, other nitrogenases model systems.

Unit IV

9. Bioredox Agents and Mechanism- Enzymes and their functioning, Vitamin B12 coenzyme, its function and application in organic syntheses, intake of alcohol and its remedy.

10. Metalloenzymes-Zinc enzymes-carboxypeptidase and carbonic anhydrase, Copper enzymes superoxide dismutase.

11. Calcium in Biology-Calcium in living cell, transport and regulation, molecular aspects of intramolecular processes.

Books Recommended:

1. Principles of Bioinorganic Chemistry, S. J. Lippard and Berg, University Science Books.
2. Inorganic Biochemistry, Vol I and II. Ed. G. L. Eichhorn, Elsevier.
3. J.E. Huheey: Inorganic Chemistry III & IV Ed. Pearson Education Asia – (2002).
4. F.A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, 5th Edition.
5. Progress in Inorganic Chemistry, Vols 18 and 38 Ed. J. J. Lippard, Wiley