बुन्देलखण्ड विश्वविद्यालय, झाँसी

सूचना

एतत् द्वारा सूचित किया जाता है कि रसायन विज्ञान पाठ्यक्रम समिति की बैठक दिनांक 02/07/2022 को अपरान्ह 12.30 बजे विश्वविद्यालय सभागार में ऑनलाइन/ऑफलाइन के माध्यम से आहूत की गयी है। अतः आपसे अनुरोध है कि बैठक में निर्धारित तिथि एवं समय पर उपस्थित होने का कष्ट करें।

कार्यसूची :-

1. उत्तर प्रदेश शासन के पत्र संख्या-नि.-401/सत्तर-3-2022 दिनांक 09/02/2022 के अनुसार उच्च शिक्षण संस्थानों मे पाठ्यक्रम पुनर्संरचना की राज्य स्तरीय समिति द्वारा प्रदेश के समस्त विश्वविद्यालयों एवं महाविद्यालयों में राष्ट्रीय शिक्षा नीति-2020 को स्नातक (शोध सहित), स्नातकोत्तर एवं पी0एच0डी0 स्तर पर लागू किये जाने हेतु सुझाव।
2. सत्र 2022-2023 की परीक्षा हेतु प्राशिनकों/ परीक्षकों की सूची तैयार करने सम्बन्धी कार्य।
3. अन्य मद अध्यक्ष की अनुमति से।

सेवा में,

1	डॉ0 सुरभि यादव, प्राध्यापक- रसायन विज्ञान विभाग, बिपिन बिहारी महाविद्यालय, झाँसी।	संयोजक
2	डॉ0 अनिल कुमार, प्राध्यापक- रसायन विज्ञान विभाग, बिपिन बिहारी महाविद्यालय झाँसी, 9450075513	सदस्य
3	डॉ0 मुहम्मद अयूब अंसारी, प्राध्यापक - रसायन विज्ञान विभाग, बिपिन बिहारी महाविद्यालय, झाँसी, 9450270110	सदस्य
4	डॉ0 माया वर्मा, प्राध्यापिका- रसायन विज्ञान विभाग, राजकीय महिला महाविद्यालय, बांदा 9956219694	सदस्य
5	डॉ0 संजय श्रीवास्तव, जीवाजी विश्यविद्यालय ग्वालियर - 9131773953	वाह्य विशेषज्ञ
6	डॉ0 ऐकता पाण्डेय, बी0 आई0 इ0 टी0 झांसी	वाह्य विशेषज्ञ
7	डा0 चित्रा गुप्ता, समन्वयक, रसायन विज्ञान विभाग, विश्वविद्यालय परिसर, झांसी	विशेष आमंत्रित सदस्य

23/6/2022

सहायक कुलसचिव
कृते कुलसचिव

बुन्देलखण्ड विश्वविद्यालय, झाँसी

पत्रांकः- बु0वि0/एके0/2022/17286-293 दिनांकः- 24.6.22

प्रतिलिपि - निम्नलिखित को सूचनार्थ एवं आवश्यक कार्यवाही हेतु प्रेषित।

1. उपर्युक्त समस्त सदस्यगण
2. अध्यक्ष, एन0ई0पी0 टास्क फोर्स।
3. संकायाध्यक्ष- विज्ञान।
4. वित्त अधिकारी।
5. सहायक कुलसचिव (अतिगोपनीय)।
6. कुलपति जी के निजी सचिव।
7. कुलसचिव के आशुलिपिक।

सहायक कुलसचिव
कृते कुलसचिव

तार : विश्वविद्यालय
Gram : UNIVERSITY

टेलीफोन : कार्या0 : 2320496
कुलसचिव : निवास : 2321214
फैक्स : 0510 : 2321667

बुन्देलखण्ड विश्वविद्यालय, झाँसी
BUNDELKHAND UNIVERSITY, JHANSI (U.P.)

झाँसी (उ.प्र.) 284128

संदर्भ...BU/Chem./2022/40 दिनाँक.....

BOARD OF STUDIES MINUTE

Board of Studies Meeting of the Department of Chemistry was conducted on 02/07/2022 at 11:30 AM in V.C. Committee room. The details of the committee members is as Below.

1. Dr. Surabhi Yadav **(Convener)**
2. Dr Anil Kumar
3. Dr. Mohammad Aqub Ansari
4. Dr. Maya Verma
5. Dr.Sanjay Srivastava **(External Expert)**
6. Dr. Ekta Pandey **(External Expert)**
7. Dr. Chitra Gupta **(Coordinator)**

Proceeding

1. A meeting of the Board of Studies (Chemistry) was held in the VC committee room regarding M.Sc. Chemistry Syllabus on 02/07/2022. As per NEP 2020 all the members and experts discussed for the revision and upgradation of M.Sc. Syllabus.

2. B.Sc./M.Sc. 2022-23, list of Examiners and Paper Setters for Practical / Theory for the Session 2022-2023 was prepared with the consent of all Board of Studies members and handed over to the Examination Cell. All the members and organizers collectively completed the task of BOS.

3. All the board of studies members coordially decided to submit the M.Sc. Chemistry revised Syllabus as per NEP 2020 to the Academic Cell of the University till 07/07/22 for further proceedings.

Report Submitted by

Dr. Chitra Gupta
(Coordinator)
Department of Chemistry
B.U.Jhansi

रसायन विज्ञान पाठ्यक्रम समिति

आज दिनांक 02/05/2022 को पूर्वाह्न 11:30 बजे विश्वविद्यालय सभागार में रसायन विज्ञान पाठ्यक्रम समिति की बैठक आहूत की गई।

उक्त बैठक में उपस्थित सदस्यों की विवरण निम्नवत है।

1. डा० सुरभी यादव
2. डा० अनिल कुमार
3. डा० मोहम्मद आयूब अंसारी
4. डा० माया वर्मा
5. डा० संजय श्रीवास्तव
6. डा० ऐक्ता पाण्डेय
7. डा० चित्रा गुप्ता

कार्यवाही

(i) आज दिनाँक 02.07.2022 को पूर्वाह्न 11:30 बजे विश्वविद्यालय सभा कक्ष में रसायन विज्ञान पाठ्यक्रम समिति की बैठक आहूत की गयी। सभी सदस्यों एवं बाह्य विशेषज्ञों के सुझाव एवं विश्व विद्यालय की नई शिक्षा पद्धति अध्यादेश 2022 के आधार पर परास्नातक रसायन विज्ञान का पाठ्यक्रम संशोधित करने पर विचार-विमर्श हुआ।

(ii) सभी सदस्यों ने सर्वसम्मति से बी.एस-सी/एम.एस-सी० वर्ष 2022-2023 की थ्योरी/प्रेक्टीकल की सूची परीक्षकों सहित तैयार कर कार्यालय को प्रेषित की गयी। सभी उपस्थित सदस्यों एवं संयोजक ने साथ मिलकर कार्य सम्पादित किया।

(iii) सर्व सम्मति से यह निर्णय लिया गया की उपरोक्त पाठ्यक्रम में संशोधन के उपरान्त दि: 07.07.2022 तक विश्व विद्यालय के अकादमिक विभाग में प्रस्तुत कर दिया जायेगा।

Convenor (Dr. M. A. Ansari)

(Dr. Maya Verma)

Dr. Chitra Gupta (Co-ordinator) Dept. of Chemistry B.U. Jhansi (U.P.)

Dr. Anil Kumar

(डा० संजय श्रीवास्तव)

तार : विश्वविद्यालय
Gram : UNIVERSITY

टेलीफोन : कार्या0 : 2320496
कुलसचिव : निवास : 2321214
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बुन्देलखण्ड विश्वविद्यालय, झाँसी

BUNDELKHAND UNIVERSITY, JHANSI (U.P.)

झाँसी (उ.प्र.) 284128

संदर्भ. Bul.Chem/2022/81

दिनाँक. 02/7/22

The Minutes of Meeting of BOS

In Reference to the BOS of Department of Chemistry Institute of Basic Science held on 02/07/2022 regarding the revision of Syllabus in tune with CBCS/NEP-2020 and subsequent approval from Academic Council. This is to certify that the Syllabus is 20% revised.

Dr. Chitra Gupta
Co-Ordinator
Department of Chemistry

Co-ordinator
Dept. of Chemistry
Bundelkhand University
Jhansi-284128 (U.P.)

ORDINANCE FOR POSTGRADUATE PROGRAMMES
(CBCS SYSTEM & NEP 2020)
ARTS, SCIENCE & COMMERCE FACULTIES
(2022 onwards)

1. INTRODUCTION

1.1 Preamble

This ordinance governs all the rules and regulations as per the NEP 2020 for the traditional post graduate programs (M.A., M.Sc., M.Com, Management courses. etc) which are not covered by any regulatory bodies (AICTE, BAR Council, PCI, NCTE etc) running in the University campus or its affiliated colleges in Bundelkhand University, Jhansi. This ordinance supersedes all the previous relevant ordinances, rules and regulations.

1.2 Duration

Bundelkhand University has adopted the CBCS system in various Postgraduate courses as per guidelines of Higher Education Department, Uttar Pradesh Government vide letter No 401/seventy-3-2022 dated 09-02-2022 to accelerate the teaching-learning process and enable vertical and horizontal mobility in learning from the academic session 2022- 23 onwards.

The duration of PG courses shall be of two years comprising of four semesters. In case a student(s) exits from this programme after completion of the first year (2 semesters), he/she may take exit from the programme and shall be awarded the Degree of Bachelor in Research. After the successful completion of two years (4 semesters) a student shall be awarded the Master's degree in the concerned subject. The maximum duration to complete the course shall be four years.

1.3 Eligibility for Admission

- Candidate, who wishes to seek admission in a course of study prescribed for a post graduate degree of the University, shall be admitted to campus or an affiliated college unless he/ she has:

  -passed the three years Bachelor's degree course Examination of the University of Uttar Pradesh or any other Indian University incorporated by any law in force at the time of admission.
  or
  -passed any other equivalent examination recognized by the University as equivalent thereto.
  -passed any other equivalent examination recognized by a Foreign University as equivalent thereto

- The date of admission shall follow the University academic calendar.

1.4 Choice of Subject and Course Structure

i. University/ College shall admit students as per the eligibility criteria and availability of seats decided by the university.

ORDINANCE FOR POSTGRADUATE PROGRAMMES
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  or
  -passed any other equivalent examination recognized by the University as equivalent thereto.
  -passed any other equivalent examination recognized by a Foreign University as equivalent thereto

- The date of admission shall follow the University academic calendar.

1.4 Choice of Subject and Course Structure

i. University/ College shall admit students as per the eligibility criteria and availability of seats decided by the university.

ii. A student shall take admission to post graduation first year of fourth year of Higher Education program of NEP 2020 after successful completion of Graduate course from NEP 2020 or old course of Science/ Arts/ Commerce/ Management, etc. He/she shall have to choose respective faculty courses as per guidelines of NEP 2020 depending on the number of seats available in concerned subject and eligibility criteria. In case a candidate is willing to change the faculty, the following conditions are required-

The candidate who has passed Bachelor degree in Science/ Commerce of NEP 2020 or old courses may take admission in some subjects of Arts faculty (excluding practical subjects like geography, psychology etc). Similarly, the Student from Commerce of NEP or old course of commerce may also be eligible to take admission in Arts subjects. Arts, Management and Commerce candidates cannot be admitted in Science subjects.

iii. Student(s) shall select subjects for Post graduation course from the major subjects that he / she had opted in the graduation course and shall continue with the same subjects in all the four semesters of the PG programme.

iv. The course structure shall be as follows:

There shall be four compulsory theory papers in the first semester. In the third and fourth semester there shall be minimum two compulsory papers and one/ two elective papers. The elective papers shall be specialization papers.

Student(s) shall have to select one open elective paper as **Minor subject** from any other faculty (except own faculty) or an interdisciplinary subject in the first semester of the first year.

v. Student(s) shall take a Research Project /Survey/ Industrial /Field training program etc. in both the years (Semester I,II,III and IV). No pre-requisite shall be required for this.

vi. List of Minor Elective Courses: The candidate shall select any one subject from the following as minor subject in first year of post graduate course.

S No	Science	Arts	Commerce	Interdisciplinary
1.	Mathematical Biology	Tribal Culture and Heritage	Customer Relationship Management	Ancient Medical Sciences
2.	Natural Resources and Conservation	Social Sector and Gender Economics	House Keeping and Hospitality	Traditional Medical Therapy
3.	Pollution: Causes and Mitigation	Socio-Economic and Social Security	Share Market and Banking	Vedic Mathematics
4.	Computational Research	Archeological Sites and Monuments	Marketing and Accounting	Medicinal and Aromatic Plants Cultivation, extraction and nutraceutical Values
5.	Data Science	Constitution of India	Insurance Policy and Finance	Disaster Management
6.	Computer Hardware Handling	Communication and Personality Development	Advertising Management	Medicinal Biochemistry
7.	Computer Software	Film, TV,	Digital	Soil and Water

	Handling	Documentary Patkatha Lekhan	Marketing	Testing
8.	Cyber Crime	Urban Growth & Development Economics	Human Resource Management	Climate Change and Environmental Degradation
9.	Bee Keeping, Aquaculture and Fish Farming	Urban Economics and Planning	Organizational Behavior	Spiritual Wellness

2. SEMESTER AND CREDIT DISTRIBUTION

An academic year for post graduate program is divided into four semesters. The Odd semesters may be scheduled from July to December and Even semester from January to June.

Fourth Year

	VII Sem	Credits	VIII Sem	Credits
Major	Theory – 04 Papers Or Theory – 04 Papers Practical -02	5 Credits each Total Credits=20 Or 4 Credits each Total Credits=16 2 Credit each Total Credits=4 **Total Credits=20**	Theory – 04 Papers Or Theory – 04 Papers Practical -02	5 Credits each Total Credits=20 Or 4 Credits each Total Credits=16 2 Credit each Total Credits=4 **Total Credits=20**
Minor	Minor Elective-1 paper of 04 credits	04 Credits **Total Credits=04**		
Research Project/ Industrial training/ Survey/ Field Training	One of each 04 Credits	04 Credits **Total Credits=04**	One of each 04 Credits	04 Credits **Total Credits=04**
Total Credits		28		24
Total in Both Semester				**52 Credit**

Fifth Year

Semester	IX	Credits	X	Credits
Major	Theory – 04 Papers Or Theory – 04 Papers Practical -02	5 Credits each Total Credits=20 Or 4 Credits each Total Credits=16 2 Credit each Total Credits=4 **Total Credits=20**	Theory – 04 Papers Or Theory – 04 Papers Practical -02	5 Credits each Total Credits=20 Or 4 Credits each Total Credits=16 2 Credit each Total Credits=4 **Total Credits=20**
Research Project / Industrial training / Survey	One of each 04 Credits	04 Credits **Total Credits=04**	One of each 04 Credits	04 Credits **Total Credits=04**
Total Credits		24		24
Total in Both Semester	**48 Credit**			

3. ATTENDANCE

The expression "a regular course of study" wherever it is used in these Ordinances, means attendance of at least 75% of the lectures and other teaching in campus / affiliated college in the subject for the examination at which a candidate intends to appear and at such other practical work (such as work in a laboratory) as is required by any Statute, Ordinance or Regulation in force for the time being in the University.

A shortage up to 5% of the total number of lectures delivered or practical work done in each subject may be condoned by the Principal of the college/ Head of the Department (in case of University Campus) concerned.

A further shortage up to 10% may be condoned only by the Vice- Chancellor on the specific recommendation of the Principal of the college/Head of the Department concerned (in case of University Campus).

4. EXAMINATION

1. There shall be examinations at the end of each semester as, for odd and even semesters in accordance with the academic calendar of the university. A candidate who does not pass the examination in any

course(s) shall be permitted to appear in such failed course(s) in the subsequent examinations upto the maximum duration of the course.

2. It is mendatory for a student to get enrolled/ registered for the first semester examination. If enrolment/ registration is not possible owing to shortage of attendance / rules prescribed OR belated joining or on medical grounds, such students shall not be permitted to proceed to the next semester. Such students shall re-do the first semester in the subsequent term of that semester as a regular student; however, a student of first semester shall be admitted in the second semester, if he/she has successfully completed the first semester.
3. It shall be mandatory for the student(s) to register for examination in each and every semester (i.e. to fill up the examination form with the requisite fee). If a student fails to register for the examination in any semester, he or she shall not be allowed to appear in the examination of that semester. Such student(s) shall appear in the (next) subsequent examination of that semester as back paper.

5. EVALUATION

The performance of a student in each course shall be evaluated in terms of percentage of marks with a provision for conversion to grade point. Evaluation for each course shall be done by a Continuous Internal Assessment (CIA) by the concerned course teacher as well as by end semester examination and will be consolidated at the end of course. The evaluation must be continuous and holistic and should be based on following parameters:

i. Academic assessment
ii. Skill assessment
iii. Physical assessment
iv. Extra-curricular assessment

5.1 THEORY PAPER

Semester Examinations shall be conducted by the university as mentioned in the academic calendar. The Question paper will be set by the examiners appointed by the Vice Chancellor based on the recommendation of the Board of Studies. The pattern of the question paper/papers may be changed /modified by Deans committee whenever required.

Internal Assessment(C.I.A.) –25%weightage of a course

- Test/ Mid-Term Assessment - 10 marks
- Term paper/Presentation on given project/assignment – 10 marks
- Attendance/activities – 05marks

ii. End Semester Exam (External examination)– 75% weightage of course

5.2 PRACTICAL PAPER

Practical examinations will be conducted by the examiners appointed by the Vice Chancellor on the recommendations of the Board of Studies. Each student has to present the practical records.

i. Internal Assessment(C.I.A.) –25%weightage of a course

- Test/ Mid-Term Assessment - 10 marks

- Term paper/Presentation on given project/assignment - 10marks
- Attendance/activities – 05marks

ii. End Semester Exam (External examination)– 75% weightage of a course

6. MINIMUM PASSING STANDARD

1. The minimum passing standard for combined external and internal examinations for each subject/paper shall be 40%,i.e. 40 out of 100 marks for theory and practical courses. The minimum passing standard for Aggregate in a semester end Examination shall be 40%.
2. Continuous Internal Assessment (CIA) shall be ensured by the Principal of the colleges / HODs for the Campus courses. The Principal of the colleges / HODs of the Campus shall provide the marks of the same to the university and it shall be mandatory to maintain the records of the same till the maximum duration of that course.
3. The internal assessment, field training and practical examination awards of a student who fails in any semester examination shall be carried forward to the next examination.
4. It shall be mandatory for a student to secure minimum 40% marks (i.e. 30/75) in the theory and (10/25) practical paper separately.

7. PROVISION FOR BACK PAPERS AND EX-STUDENTS

A Back Paper (B.P.) candidate shall be promoted to the next semester. The back paper facility in a semester provides promotion to the next semester and another opportunity to obtain a minimum of the pass marks assigned for an individual paper or in the aggregate. Following category of students of Bundelkhand University shall be eligible for back paper facility as under

1. A student shall be required to pass in minimum two subject papers in each semester. However, at the end of each year, it shall be mandatory for a student to pass in at least two subjects/ papers and minor paper otherwise he/she shall be deemed as failed and will be treated as a year back / ex- student.
2. Students shall get the attempts to appear in the Back paper examination in the subsequent odd /even semester till the maximum duration of the said course.
3. Special back paper examination shall be held only for regular students of the final year of PG course.
4. The candidate, who fails in more than three of the total papers, will be deemed as failed. These candidates can appear only in subsequent examination of that semester as Ex-Students.

8. PROMOTION RULES

8.1 Semester Course & Examination

The students who have taken admission in any post-graduation programme in a session and who have put in the minimum percentage of attendance for appearing at the Examination, presented himself/herself for internal assessment and have filled in the examination form in time for appearing at the End Semester Examination shall be allowed to appear at the respective examinations.

8.2 Declaration of Results

After appearing in the Examination of both the semesters in a particular year, the student can be put in the following categories in the context of declaration of the results of the Semester Examination:

Passed
Promoted with Back Paper(s)
Failed

8.3 Promotion to Next Semester

All students under category Passed and promoted with back papers shall be promoted to the next Semester (as mentioned in Point 7)

"Failed" students may clear their UNCLEARED courses in subsequent examinations as ex-students.

Students promoted with back papers shall clear their back papers in subsequent examinations as ex-students.

A student who has failed in a course shall get two more chances to clear this course subject to the maximum duration for passing the course. Further, each candidate shall have to clear all the courses within the maximum period of four years from the date of his/her latest admission.

A candidate who has qualified for the Degree shall be placed in the First / Second Division as per following table:

8.4 Computation of SGP and CGPA

The guidelines formulated by Bundelkhand University shall be followed in order to bring uniformity in evaluation system of every CBCS based Course and computation of the SGPA (Semester Grade Point Average) and CGPA (Cumulative Grade Point Average) based on students' performance in examination. The number of core, elective, open elective papers (Minor) and the required credit for each paper shall be formulated by respective Board of Studies (BOS). For the purpose of computation of work load the UGC proposed mechanism is adopted i.e. one credit=1 Theory period of one hour duration, 1credit= 1Tutorial period of one hour duration, 1credit=1 Practical period of one hour duration. The credit(s) for each theory paper/practical/tutorial/dissertation will be as per the respective Board of Studies of departments.

Letter Grade	Numerical grade
O (outstanding)	10
A+ (Excellent)	9
A(very good)	8
B+(Good)	7
B(average)	6
F(Fail)	<4
Ab (Absent)	0

The minimum passing marks shall be 40%of the maximum marks as prescribed in the University Examination and 40%of marks in the aggregate marks in the subject including internal / sessional marks.i.e. Minimum Passing Grade is "B".

A student who obtains Grades "O"or"B" shall be considered as PASSED. If a student secures "F" grade, he/she shall be considered as FAILED and shall have to re appear in the examination. It is

mandatory for a student to earn the required SGPA as in each semester. If a student is not able to secure 40% / B grade in any theory / practical / internal / sessional / viva-voce / internship / project examination, the awarded grade point shall be ZERO (0).

8.5 The University, adopts absolute grading system where in the marks are converted to grades, and every semester results will be declared with semester grade point average (SGPA). The Cumulative Grade Point Average (CGPA) will be calculated in end of final semester. The grading system except pharmacy department will be with following letter grades and grade points scale as given below:

Table

Level	Outstanding	Excellent	Very Good	Good	Average	Fail
Letter Grade	O	A+	A	B+	B	F
Grade Points	10	9	8	7	6	0
Score (Marks) Range (%)	≥90 (90-100)	<90, ≥80 (80-89.99)	<80, ≥70 (70-79.99)	<70, ≥60 (60-69.99)	<60, ≥40 (40-59.99)	<40 (0-39.99)
Award	**First Division with Distinction**		**First Division**		**Second Division**	**Fail**

1. A student obtaining Grade "F" shall be considered failed and will be required to reappear in the examination. Such students after passing the failed subject in subsequent examination / will be awarded with grade respective of marks he/she scores in the subsequent examination/s.
2. The University has the right to scale/moderate the theory exam / practical exam / internal exam / sessional marks of any subject when ever required for converting of marks into letter grades on the basis of the result statistics of university as in usual practice, i.e. marks obtained in decimal will be converted in nearest integer.

9 CONVERSION OF GRADES IN TO PERCENTAGE

Conversion formula for the conversion of CGPA into Percentage is
CGPA Earned **x 9.5 = Percentage of marks scored.**

Illustration: CGPA Earned 8.6 x 9.5 = 82.0%

10. UNFAIR MEANS

Cases of unfair means in the End Semester Examinations and Mid-Term Tests shall be dealt as per the rules laid by the University.

Note:

1. Those students who are NOT eligible for promotion to next year shall have to reappear in the coming examination as ex-students. However, the marks of internal assessment shall be carried forward in such cases.

2. Scrutiny facility and Challenge evaluation facility shall be available for those students who want to improve their grades.

Programme Overview

M.Sc. (Chemistry)

Department of Chemistry, Bundelkhand University Jhansi, is well updated M.Sc. Chemistry syllabus as per NEP-2020. It aims to develop young talents for scientific research, chemical industry and education. The curriculum is developed in such a way that the students are able to venture into allied fields as well. Through the courses offered by the department, the department aims to provide "a cut above the rest" man-power for the growing demands of the industry and prepare the students for higher studies and research. The interactive method of teaching in the Department of Chemistry is meant to bring about behavioral change for the future professionals of the industry. Equal importance is given to practical and theoretical methods of learning apart from experiential and digital methods of learning. Industrial projects form an integral part of the curriculum. Apart from the curriculum, the university lays emphasis on value addition programs like Current Affairs, Holistic Education, Certificate Courses and Placement Training Programs which include training the students in group discussions, face to face interviews etc. We have a diverse student population with representation from almost all states in India and abroad. The department is blessed with highly qualified faculty members who come from diverse backgrounds and are involved in cutting edge research in various subject areas as well as in interdisciplinary areas. The curriculum is frequently revised and provides opportunities for projects and joint research with faculty members.

Apart from curricular subjects, the department offers personality development and society-oriented programmes, career guidance, placements, and opportunities to participate in competitions, seminars and conferences. Our commitment to excellence in teaching and research has helped graduate students from the department achieve distinction in academia and industry.

Program Outcomes(POs)

PO1: Creative Thinking: Students will be able to think creatively (divergent and convergent) propose new ideas to explain facts and figures or provide new solutions to problems problems in chemistry. Drawing skills and logical conclusions from observations scientific experiments will also develop.

PO2: Interdisciplinary Approach: Students will feel how development takes place in any science. The subject helps in the development of other science subjects and vice versa and how Interdisciplinary approach helps to provide better solutions and new ideas for sustainable Events. as well as knowledge of subjects in other faculties such as humanities, performance arts, social science etc. can have immense and effective influence which motivates to develop New scientific theories and inventions.

PO3: Personality Development: Students will imbibe moral, ethical and social values Personal and social life leads to a highly cultured and civilized personality. they will also Realize that the pursuit of knowledge is a lifelong activity and that it is in combination with tireless efforts and positive attitude and other essential qualities lead to a successful life.

PO4: Skills in Research and Industry: Scientific temper will be inculcated in students and will be able to learn the skills needed to be successful in the research or industrial sector. besides they will acquire skills in handling, planning and performing scientific equipment in the laboratory Experiment.

PO5: Communication Skills: Students will develop various communication skills such as reading, listening, speaking etc., which will help us to express thoughts and ideas clearly and Effectively.

PO6: Environmental Monitoring: Students will be able to understand environmental issues will create awareness in global warming, climate change, acid rain, ozone depletion and community.

Program Specific Outcomes (PSOs)

PSO-1 Students will understand the basic concepts, fundamental principles, and the scientific theories related to various scientific phenomena and their relevancies in the day-to-day life. They will also be able to acquire knowledge about the fundamentals and applications of chemical and scientific theories.

PSO-2 Students will find that every branch of science and technology is related to Chemistry. They will develop scientific outlook not only with respect to science subjects but also in all aspects related to life.

PSO-3 Students will become familiar with the different branches of chemistry like analytical, organic, inorganic, physical, environmental, polymer and biochemistry. They will also learn to apply appropriate techniques for the qualitative and quantitative analysis of chemicals in laboratories and in industries.

PSO-4 The student will acquire knowledge of Chemical Thermodynamics, Kinetics, Electrochemistry, Atomic Structure, Organic Chemistry, Spectroscopy and Skill in Industrial Chemistry.

PSO-5 Viewing chemistry as a tool the developing mind and critical attitude and the faculty of logical reasoning that is prepared to serve in diverse fields.

PSO-6 Students will gain a thorough Knowledge in the subject to be able to work in projects at different research as well as academic institutions

Course Structure For M.Sc. Chemistry (VII-X Semester)

SEMESTER	PAPER CODE	PAPER	THEORY (MARKS-75 MAX.)	INTENRAL (MARKS - 25)			CREDIT
			75	25*			
			75	10	10	5	
VII	CHY 701	Application of Computer in Chemistry	75				4
	CHY 702	Inorganic Chemistry	75				4
	CHY 703	Organic Chemistry	75				4
	CHY 704	Physical Chemistry	75				4
	CHY 705	Minor Elective Course	75				4
	CHY 706	Practical (Organic, Inorganic, & Physical Chemistry)	75				4
	CHY 707	Research Project/Industrial & field Training/ Survey	100	-	-	-	4
VIII	CHY 801	Inorganic and Group Theory	75				4
	CHY 802	Organic Chemistry	75				4
	CHY 803	Physical Chemistry	75				4
	CHY 804	Spectroscopy	75				4
	CHY 805	Practical (Inorganic, Organic, & Physical Chemistry)	75				4
	CHY 806	Research Project/Dissertation (continue 707)	100	-	-	-	4
IX	CHY 901	Application of spectroscopy	75				4
	CHY 902	Biochemistry	75				4
	CHY 9031-9034	Paper Elective	75				4
	CHY 9041-9044	Paper Elective	75				4
	CHY 905	Practical (Organic, Inorganic, & Physical Chemistry)	75				4
	CHY 906	Research Project/ Industrial & field Training/ Survey	100	-	-	-	4
X	CHY 1001	Photochemistry/ Solid State	75				4
	CHY 1002	Environmental chemistry	75				4
	CHY 10031-10034	Paper Elective	75				4
	CHY 10041-10044	Paper Elective	75				4
	CHY 1005	Practical (Instrumental methods of Analysis and Organic Synthesis)	75				4
	CHY 1006	Project/Dissertation	100	-	-	-	4
		Grand Total	**2500**				**100**

Note: Duration of practical examination shall be 16 Hrs. (8 Hrs. / day) in each semester *****Internal assessment 25% weightage of a course which includes 10 Marks mid-term assessment, 10 marks assignment/ presentation of given project and 5 marks of attendance/ activities.

SEMESTER – VII

Paper -1

M.Sc. VII Semester

CHY-701: Application of Computer in Chemistry

Paper Type: Theory Total Hours: 60

Paper type: Core Total Credits: 4

Objective:

The objective of the course is to help the students learn the basics of computers to deal with text formatting, statistical analysis, presentations and writing programs to solve various chemical equations.,

Course Outcomes:

After successful completion of this course, students will be able:

CO1: Learn the fundamentals of computer systems and its components.

CO2: Work on word processor and create well formatted documents. create spreadsheets and employ basic functions, create charts, perform statistical analysis.

CO3: learn programming in chemistry and write programs for solving chemical equations.

CO4: Learn Monte Carlo and molecular dynamics, programs with data preferably from physical chemistry laboratory, further, the students will operate this program in chemistry.

CO5: Development of small computer codes involving simple formulae in chemistry, such as Vander Waals equation, pH titration, kinetics etc.

Unit-1: Introduction to computers and computing: Basic structure and functioning of computers with a PC as an illustrative example, Memory, I/O devices, secondary storage, computer language, operating systems with DOS as an example, introduction to UNIX and WINDOWS, data processing, principles of programming, algorithms and flow-charts. **8**

Unit-2: Computer programming in FORTRAN / Basic: Elements of the computer language, constants and variables, operations and symbols, expressions, arithmetic assignment statement, input and output. Format statement, termination statements, and branching statements such as IFor GO TO statement. Logical variables double precision variables, subscribed variables and Dimension, DO statement, FUNCTION and SUBROUTINE, COMMON and DATA statements. **12**

Unit-3: Programming in Chemistry: Development of small computer codes involving simple **15**
formulae in chemistry, such as Vander Waals equation, pH titration, kinetics, radioactive decay, evaluation of lattice energy and ionic radii from experimental data,linear simultaneous equations to solve secular equations within the Huckel's theory, elementary structural features such as bond lengths, bond angles, dihedral etc of molecules extracted from a database such as Cambridge data base.

Unit-4: Use of Computer Programs: The students will learn how to operate a PC and how to **25**
run standard programs and packages, execution of linear regression, X-Y plot, numerical integration and differentiation as well as differential equation solutionprogramms, Monte Carlo and molecular dynamics, programs with data preferably fromphysical chemistry laboratory, further, the students will operate one or two or thepackages such as MATLAB, EASYPLOT, LOTUS, FOXPRO, FOXPRO and Wordprocessing software such as WORDSTAR/MS-WORD.

Books Recommended

i. **R. Hunt and J. Shelley,** *"Computers and Common Sense"*, Prentice Hall,

ii. **A.C. Norris** *"Computational Chemistry"*.

iii.**J.P. Kilingbeck and Adam Hilger**, *"Microcomputer Quantum Mechanics"*.

iv.**V. Rajaraman,** *"Computer Programming in FORTRAN IV",* Prentice Hall.

v. **V. Rajaraman and T. Radhakrishnan,** *"An Introduction to Digital Computer Design",* Prentice Hall.

vi. **V. Rajaraman,**"*Fortran 77"*, Prentice Hall (India), New Delhi (1997)

vii. **C. Xavier,** *"Fortran 77 and Numerical Methods",* New Age International Pvt. Ltd. Publishers,New Delhi (1994)

viii. **S. Lipschutz and A. Poe, Schaum's** *"Outline Series – Theory and Problems of Programming with Fortran including structured Fortran*", Mc Graw Hill Book Company, Singapore (1982)

ix. **K. V. Raman,**"*Computers in Chemistry",* Tata McGraw Hill (1993). [Reference book].

Paper -2

CHY-702: Inorganic Chemistry

Paper Type: Theory Total Hours: 60

Paper type: Core *Total Credits: 4*

Objective:

Understanding structure, bonding and reaction mechanism involved in inorganic solids, mwtal ligand bonding and metal pi-complexes. Applying practical aspects of inorganic chemistry in research and development.

Course Outcomes:

After successful completion of this course, students will be able:

CO1: Stereochemistry and Bonding: Compare trends in the properties of main group elements and discuss mechanisms of inorganic reactions.

CO2: Examine and apply the stability of metal complexes with reference to the nature of metral ion and ligand.

CO3: Discuss the concepts of organometallic and nuclear chemistry 6. Justify the implication of nuclear chemistry in energy generation

CO4: The students will be able to pursue their career in higher education, scientific research and teaching.

Unit-1: Stereochemistry and Bonding in Main Group Compounds: 12

VSEPR, Walsh diagram (tri- and penta- atomic molecules), d_{π}-P_{π} bonds, Bent rule and energetic of hybridization, Reactions of atomic inversion, free radical mechanism, nucleophilic displacement, perry-pseudo rotation of covalently bonded molecules.

Unit-2: Metal - Ligand Equilibria in Solution: 8

Stepwise and overall formation constants 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-metry and spectrophotometry.

Unit-3: Metal-Ligands Bonding: **15**

Crystal field splitting in an octahedral and tetrahedral field, factors affecting the crystal field stabilizing energy, consequence of crystal field splitting, Dynamic & Static John-Teller Effect, Application and Limitation of crystal field theory, Site selection in spinals, molecular orbital theory, octahedral, tetrahedral and square planar complexes, π -bonding in octahedral complexes.

Unit-4: Metal π-Complexes: **18**

Metal carbonyls, structure and bonding, vibrational 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 ligands.

Unit-5: Bonding in metal: **7**

Introduction, Classical free electron theory, Molecular orbital approach,Valence bond approach, metallic conductivity, collision energy, metallic radii, distribution of metallic properties.

Books Recommended

1. **F.A. Cotton and G. Wilkinson**, "*Advanced Inorganic Chemistry"*, 6thEdn. (1999), John Wiley & Sons, New York.
2. **J.E. Huheey, E.A. Keiter and R.L. Keiter**, "*Inorganic Chemistry"*, 4th Edn. (1993), Addison-Wesley Pub. Co., New York.
3. **R. S. Drago,**"*Physical Methods in Inorganic Chemistry"*, International Edn. (1971), Affiliated East-West Press, New Delhi.
4. **Keith F. Purcell and John C. Kotz**, "*Inorganic Chemistry",* W. B. Sauders Com. (1987), Hong Kong.
5. **K. Veera Reddy,**"*Symmetry and Spectroscopy of Molecules"*, New Age International Pvt. Ltd., New Delhi (1999).
6. **B.N. Figgis,**"*Introduction to Ligand Fields",* Wiley Eastern Ltd. New Delhi (1976).
7. **R.L. Carlin,** "*Magnetochemistry"*, Springer Verlag.
8. **G. Wilkinson, R.D. Gillars and J.A. McCleverty,** "*Comprehensive Coordination Chemistry*", eds.Pergamon.

Paper -3

CHY-703: Organic Chemistry

Paper Type: Theory Total Hours: 60

Paper type: Core *Total Credits: 4*

Objective:

on completion of this course students will be able to apply the concepts of bonding , aromaticity, stereochemistry, reaction mechanism and different types of stereochemical reactions.

Course Outcomes:

After successful completion of this course, students will be able:

CO1: Nature of bonding in organic molecules, concept of aromaticity , antiaromaticity and homo aromaticity with different examples.

CO2 : Stereochemistry- All concepts including stereospecific and stereoselective synthesis, asymmetric synthesis, optical activity in the absence of chiral carbon along with stereochemistry of compounds containing nitrogen , sulphur and phosphorus.

CO3: Reaction mechanism: Structure and reactivity, Physical organic chemistry which wll help students to understand basics of organic chemistry and new approaches in the Organic Chemistry

CO4: This course aims at explaining the different types of pericyclic reactions, the stereochemistry of the same and simple rules to predict the feasibility of the reaction and the stereochemical outcome.

Unit-1: Nature of bonding in organic molecules: 10

Delocalized chemical bonding-conjugation,cross conjugation, resonance, hyperconjugation, bonding in fullerenes, tautomerism, aromaticity in benzenoid and non- benzenoid compounds, alternant and non-alternant hydrocarbons, Huckel's rule, energy level of π -molecular orbitals, annulenes, anti-aromaticity, homo-aromaticity, PMO approach, bonds weaker than covalent – addition compounds, crown ether complexes and cryptands, inclusion compounds, cyclodextrins, catenanes and rotaxanes.

Unit-2: Stereochemistry: 15

Conformational analysis of cycloalkanes, decalins, effect of conformation on reactivity. Conformation of sugar, steric strain due to unavoidable crowding, elements of symmetry, chirality,

molecules with more than one chiral center, threo and erythro isomers, methods of resolution, optical purity, enantiotopic and diastereotopic atoms, groups and faces, stereospecific and stereoselective synthesis, asymmetricsynthesis, optical activity in the absence of chiral carbon (biphenyls, allenes and spiranes), chirality due to helical shape, stereochemistry of the compounds containing nitrogen, sulphur and phosphorus.

Unit-3: Reaction mechanism- Structure and reactivity: 15

Types of mechanisms, types of reactions, thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammond's postulate, Curtin-Hammett principle, potential energy diagrams, transition states and intermediates, methods of determining mechanisms, isotope effects, hard and soft acids and bases, generation, structure, stability and reactivity of carbocations, free radicals, carbenes, benzynes and nitrenes, effect of structure on reactivity-resonance and field effects, steric effect, quantitative treatment, the Hammett equation and linear freeenergy relationship, substituent and reaction constants, Taft equation

Unit-4: Pericyclic Reactions: 20

Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3butadiene, 1,3,5-Hexatriene and allyl system, classification of pericyclic reactions, Woodward-Hoffmann correlation diagrams, FMO and PMO approach, Electrocyclic reactions-conrotatory and disrotatory motions, 4n and 4n + 2 systems, 2 + 2 addition of ketenes, 1, 3dipolar cycloaddition and cheleotropic reactions. Sigmatropicrearrangements- suprafacial and antarafacial shifts of H, sigmatropicshiftsinvolving carbon moieties, 3,3-and 5,5-sigmatropic rearrangements, claisen, cope and aza- cope rearrangements, fluxional tautomerism, Enereaction.

Books Recommended

1. **Jerry March,** "*Advanced Organic Chemistry-Reactions, Mechanism and Structure",* John Wiley.
2. **F. A. Carey and R. J. Sundberg, Plenum,**"*Advanced Organic Chemistry*".
3. **C. K. Ingold,***"Structure and Mechanism in Organic Chemistry",* Cornell University Press.
4. **R. T. Morrison and R. N. Boyd,***"Organic Chemistry",* Prentice-Hall. 5.
5. **H. O. House, Benjamin,***"Modern Organic Reactions".*
6. **R. O. C. Noman and J. M. Coxon,***"Principles of Organic Synthesis",* Blackie Academic & Professional
7. **D. Nasipuri,***"Stereochemistry of Organic Compounds",* New Age International.
8. **P.S. Kalsi,** *"Stereochemistry of Organic Compounds",* New Age International.
9. **Clayden, Greeves, Warren and Wothers,***"Organic Chemistry"*, Oxford University Press, 2001.

M.B. Smith & Jerry March, "*March's Advanced Organic Chemistry"*, 5th Edition (2001), John Wiley

Paper -4

CHY-704: Physical Chemistry

Paper Type: Theory Total Hours: 60

Paper type: Core Total Credits: 4

Objective:

Physical chemistry are focused on understanding the macro and microscopic properties. Their discoveries are based on understanding chemical thermodynamics, statistical thermodynamics and quantum chemistry describing their behavior using theories of physics and mathematical computations

Course Outcomes:

After successful completion of this course, students will be able:

CO1: This course deals with basic rules and mathematical concept of physical chemistry.

CO2: This chapter deals with different types of quantum particles like boson, fermion. This is very fundamental in nature and can be studied in particle physics.

CO3: Understand of the laws of thermodynamics and their applications and to determine molar conductivity of a strong electrolyte at different concentrations and verify Debye-Hückel-Onsager equation.

CO4: Students come to know about classical thermodynamics, statistical thermodynamics, phase equillibria and thermodynamics of biological systems.

CO5: know the phase diagram of three component systems and second order phase diagram.

CO6: Understand of the quantum chemistry of free electron and H- atom. To understand and appreciate the quantum mechanical approach to the atomic and molecular electronic structure.

CO7: understand operator and application of Schrödinger wave equation.

Unit-1: Mathematical Concept for Physical Chemistry 10

- **A.** Basic rules of differentiation, integration and logarithm
- **B.** Partial differentiation
- **C.** Exact and inexact differentiation with their applications in thermodynamic properties
- **D.** Addition and multiplication of Matrix
- **E.** Permutation and Combination.
- **F.** Probability

Unit-2:Quantum Chemistry 25

A.Introduction to exact quantum mechanical results: The Schrodinger equation and the postulates of quantum mechanics, discussion of solutions of the Schrodinger equation to some model systems viz., particle in a box, the harmonic oscillator, the rigid rotor, the hydrogen atom.

B. Approximate methods: The variation theorem, linear variation principle, perturbation theory (first order and non-degenerate). Applications of variation method andperturbation theory to the helium atom.

C.Angular momentum: Ordinary angular momentum, generalized angular momentum, Eigen functions for angular momentum, Eigen values of angular momentum, operator using ladder operators, addition of angular momenta, spin, anti-symmetry and Pauli's exclusion principle.

D. **Electronic structure of atoms**: Electronic configuration, Russell- Saunders terms and coupling schemes, Slater-Condom parameters, term separation energies of the p^n configuration, term separation energies for the d^n- configurations, magnetic effects: spin-orbit coupling and Zeeman splitting, introduction to the methods of self-consistent field, the virial theorem.

E. Molecular orbital theory: Huckel theory of conjugated systems, bond order and Charge density calculations, applications to ethylene, butadiene, cyclopropeneyl radical, cyclobutadiene etc, introduction to external Huckel theory.

Unit-3:Thermodynamics: 25

Classical thermodynamics: Brief resume of concepts of laws of thermodynamics, free

energy, chemical potential and entropies, partial molar free energy, partial molar volume and partial molar heat content and their significances, determinations of these quantities, concept of fugacity and determination of fugacity. Non-ideal systems: Excess functions for non-ideal solutions, activity, activity coefficient, Debye-Huckel theory for activity coefficient of electrolytic solutions, determinations of activity and activity coefficients, ionic strength, application of phase rule to three component systems, second order phase transitions.

Statistical thermodynamics: Concept of distribution, thermodynamic probability and most probable distribution, Ensemble averaging, postulates of ensemble averaging, canonical, grand

canonical and micro canonical ensembles, corresponding distribution laws (Using Lagrange's method of undetermined multipliers), partition functions- translational, rotational, vibrational and electronic partition functions, calculation of thermodynamic properties in terms of partition functions, applications of partition functions, heat capacity behavior of solids- chemical equilibria and equilibrium constant in terms of partition functions, Fermi-Dirac statistics, distribution law and applications to metal, Bose- Einstein statics-distribution law and application to helium.

Non Equilibrium thermodynamics: Thermodynamic criteria for non- equilibrium S tates, entropy production and entropy flow, entropy balance equations for different irreversible processes (e.g. heat flow, chemical reaction etc), transformations of the generalized fluxes and forces, non-equilibrium stationary 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. **P.W. Atkins,** *"Physical Chemistry*", ELBS. , 8th Edition., Oxford University Press, New York.
2. **A.K. Chandra**,*"Introduction to Quantum Chemistry"*, Tata McGraw Hill,
3. **Ira N. Levine,***"Quantum Chemistry"*, Prentice Hall. 5th Edition., Tata McGraw Hill Pub.Co.Ltd., New Delhi.(2000).
4. **R. McWeeny**, "Coulson's Valence", ELBS.
5. **K.J. Laidler,***"Chemical Kinetics",* 3rd Edition, Harper & Row, New York (1987).

Additional References

1.P.W. Atkins and R.S. Friedman, "*Molecular Quantum Mechanics"*, 3rd edition (1997), Oxford University Press. Oxford.

2.H. Eyring, J. Walter and G.E. Kimball,"*Quantum Chemistry"*, (1944) John Wiley, New York.

2. A. Szabo and N. S. Ostlund, *"Modern Quantum Chemistry: Introduction to Advanced Electronic Structure*, (1982), Dover, New York.

Paper -5

CHY-705: Climate Change and environmental degradation

Paper Type: Theory Total Hours: 60

Paper type: Minor Total Credits: 4

Objective:

To study climate change and degradation.

Course Outcomes:

After successful completion of this course, students will be able:

CO1: know the effects of climate change on the natural environment .

CO2: understand how climate change can lead to habitat destruction and how habitat destruction can interact with other aspects of climate change to threaten the survival of some animal species.

CO3: understand how climate change has the potential to increase air pollution with potentially life-threatening consequences.

CO4: understand how climate change can worsen soil erosion and result in further climate change

CO5: Identify how systems work by looking at the relationships between climate and other forms of environmental change.

BUNDELKHAND UNIVERSITY, JHANSI
SYLLABUS FOR POSTGRADUATE COURSES M.Sc.

CLIMATE CHANGE AND ENVIRONMENTAL DEGRADATION

Total Credits: 4

Unit I: Introduction

Climate in the spotlight climate and weather, climate of India, Natural greenhouse effect, climate change factors – Natural factor &Anthropogenic factor.

Unit II: Global warming

Greenhouse gases: role of CO_2,role of CH_4, Global warming potential, CO_2 Emission – human Emission of CO_2, Remedial measure to reduce global warming, Global cooling.

Unit III: Ozone Layer Depletion

Vienna convention on the protection of ozone layer – 1985, Montreal protocol, protection and maintenance of ozone layer, Indian efforts for ozone layer protection. El-Nino and its effects, La-Nina, impact of climate change on India.

Unit IV: Sustainable Development

Brundtland Commission, UN Environmental Agenda, role of U.N. agencies, World Environment Organization, climate change convention-1992, Earth Summit, Agenda 21, IPCC, Global Environment Facility.

Unit V: Impact of Climate Change and Global Warming

Impact of Climate Change in India: Pattern change of Rainfall, Drought, Effects on water resources, Sea Level Rise, Impacts on Agriculture, Impacts on food security, Impacts on Glacier, Impacts on Health, Impacts on energy security, Impacts on Biodiversity.
Climate change & disaster in India, Urban flood, Cyclone, Forest fire

Suggested Readings:

1. **Encyclopedia of Global Warming and Climate Change** By George Philander, SAGE Publications Inc; First edition, 2008.
2. **Atmosphere, Weather and Climate** *ByRoger G. Barry, Richard J Chorley, CRC Press, 2010.*
3. **Global Warming: The Complete Briefing** By John Houghton, Cambridge University Press; 4th edition 2009.

Practical

VII Semester

CHY-706: Practical (Organic, Inorganic, & Physical Chemistry)

Paper Type: Practical Total Hours: 270

Paper type: Core Total Credits: 4

Objective:

The objective of laboratories is an important and ever-evolving topic of discussion amongst student and laboratory staff. It is often assumed that both teaching staff and students are implicitly aware of instrument and reagent. Applying practical aspects of inorganic chemistry in research and development

Course Outcomes:

After successful completion of this course, students will be able:

CO1: Discuss laboratory safety, material safety data sheet and prevention of accident & first aid measurement.

CO2: Chromatographic separation of metal ions .

CO3: Determine the distribution coefficient of iodine in different solvents.

CO4: Analyze primary binary mixtures of organic compounds.

CO5: Separation of cations and anions by paper and column chromatography.

1. Inorganic Chemistry:

A.Lab Safety:

(i) Symbols of chemical bottles.

(ii) Material Safety Data Sheet (MSDS).

(iii) CAS (Chemical Abstract Service) number.

(iv) Prevention of accident & first aid measurement.

B. Qualitative and Quantitative Analysis:

(i) Less common metal ions - TI, Mo, W, Ti, Zr, Th, V, U (two metal ions in cationic/anionic forms)

(ii) Insoluble-oxides, sulphates and halides

C. Chromatography: Separation of cations and anions by-

(i) Paper Chromatography (ii) Column Chromatography-Ion exchange.

2.Organic Chemistry

A.Qualitative Analysis:

Separation, purification and identification of compounds of binary mixture (oneliquid and one solid) using TLC and column chromatography, chemical tests. IR spectra to be used for functional group identification.

B.Quantitative Analysis:

(i) Determination of the percentage or number of hydroxyl groups in an organic compound by acetylation method. (ii) Estimation of amines/phenols using bromated bromide solution/or acetylation method.

3.Physical Chemistry
Chemical Kinetics:

(i) Determination of the effect of (a) Change of temperature, (b) Change of concentration of reactants and catalyst, and (c) Ionic strength of the media on the velocity constant of hydrolysis of an ester/ionic reactions.

(ii) Determination of the velocity constant of hydrolysis of an ester/ionic reaction in micellar media.

(iii) Determination of the rate constant for the oxidation of iodide ions by hydrogen peroxide studying the kinetics as an iodine clock reaction.

(iv) Determination of the primary salt effect on the kinetics of ionic reactions and testing of the Bronsted relationship (iodide ion is oxidised by per-sulphate ion).

(v) Oscillatory reaction.

Books Recommended

i. **J. Derek Woollins,** *"Inorganic Experiments"*, VCH.

ii. **Z. Szafran, R. M. Pike and M. M. Singh,** *"Microscale Inorganic Chemistry",* Wiley.

iii. **G. Marr and B. W. Rockett, Van Nostrand ,** *"Practical Inorganic Chemistry"*.

iv. **J. Bassett. R.C. Denney, G.H. Jeffery and J. Mendham,** *"Vogel's Textbook of Quantitative*

Analysis", revised, ELBS.

v. **W.L. Jolly,** *"Synthesis and Characterization of Inorganic Compounds"*, Prentice Hall.

vi. **D. Pasto, C. Johnson and M. Miller,***"Experiments and Techniques in Organic Chemistry"*, Prentice Hall.

vii. **K.L. Williamson, D.C. Heath,***"Macroscale and Microscale Organic Experiments"*.

viii. **H. Middleton,** *"Systematic Qualitative Organic Analysis"*Adward Arnold.

ix. **H. Clark,** *"Handbook of Organic Analysis, Qualitative and Quantitative",*Adward Arnold.

x. **A.R. Tatchell ,***"Vogel's Textbook of Practical Organic Chemistry",* John Wiley.

xi. **A.M. James and F, E. Prichard**, *"Practical Physical Chemistry"*, Longman.

xii. **B.P. Levitt***"Findley's Practical Physical Chemistry",* Longman.

xiii. **R.C. Dasand and B. Behera,***"Experimental Physical Chemistry",* Tata Mc Graw Hill.

Marks Distriution		**Max. Marks**
1.	Inorganic Experiment	20
2.	Organic Experiment	20
3.	Physical Experiment	20
4.	Record	8
5.	Viva- voce	7
		Total- 75

SEMESTER – VIII

Paper -1

CHY-801: Inorganic Chemistry

Paper Type: Theory Total Hours: 60

Paper type: Core *Total Credits: 4*

Objective:

The objective of the core paper Electronic spectra and magnetic properties of transition metal complexes focuses on charge transfer spectra, spectroscopic method of assignment of absolute configuration.

Course Outcomes:

After successful completion of this course, students will be able:

CO1: Study kinetics and mechanism of substitution reactions in Co (III) Octahedral, Tetrahedral and square planar Pt (II) complexes.Electron Transfer Reactions of metal complexes

• CO2: Study Orgel and Tanabe-Sugano Diagram (d1-d9) complexes.

• CO3: Study HNCC and LNCC carbonyl, Boranes and Carboranes and metal halide cluster.

• CO4: Study Elements of Symmetry and Point Groups ,Understand multiplication tables, irreducible representations, orhtogonality Theorem. ,Understand Matrix Representations of symmetry elements, transformation matrices , Cartesian coordinate and internal coordinate methods of normal mode analysis for different point groups

Unit-1: Reaction mechanism of transition metal complexes: Energy profile of a reaction, **20**

reactivity of metal complexes, inert and labile complexes, kinetic application of valence bond and crystal field theories, kinetics of octahedral substitution, acid hydrolysis, factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism, direct and indirect evidences in favor of conjugate mechanism, anationreactions, reactions without metal ligand bond cleavage, substitution reactions in square planar complexes, the trans effect, mechanism of the 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.

Unit-2: Electronic spectra and magnetic properties of transition metal complexes: **18**

Spectroscopic ground states, correlation, Orgel and Tanabe–Sugano diagrams for

transition metal complexes (d^1-d^9 states), calculations of Dq, B and β parameters, charge transfer spectra, spectroscopic method of assignment of absolute configuration in optically active metal chelates and their stereochemical information, anomalous magnetic moments, magnetic exchange coupling and spin crossover.

Unit-3: Metal-Clusters: Higher boranes, carboranes, metalloboranes and metallocarboranes, **12** metal carbonyl and halide clusters, compounds with metal-metal multiple bonds.

Unit-4: Symmetry and group theory in chemistry: symmetry elements and symmetry **10**

operation, definition of group, subgroup, relation between orders of a finite group and its subgroup, conjugacy relation and classes, point symmetry group, shooflies symbols, group multiplication table, representations of groups by matrices (representation for the C_n, C_{nv}, C_{nh}, D_{nh}etc groups to be worked out explicitly). character tables and their use, spectroscopy.

Books Recommended

i. **J.D. Lee**, *"Concise Inorganic Chemistry*", Fifth Edition,(2016),John Wiley & Sons,New York.

ii. **J.E. Huhey, Ellen A. Keiter, Richard L. Keiter and Okhil K. Medhi**,"Inorganic Chemistry, Principles of Structure and Reactivity", Fourth Edition, Pearson.

iii. **N.N. Greenwood and A. Earnshow,** *"Chemistry of the Elements",* Pergamon.

iv. **A.B.P. Lever,***"Inorganic Electronic Spectroscopy"*, Elsevier.

v. **R.L. Carlin,***"Magnetochemistry"*, Springer Verlag.

vi. **F. A. Cotton,** "*Chemical Applications of Group Theory"*, 3rd Edn. (1999), John Wiley & Sons, New York.

vii. **D.A. Mc Quarrie and J.D. Simon,***"Physical Chemistry: A Molecular Approach"*, (1998) Viva Books,New Delhi.

viii. **G. Wilkinson, R.D. Gillars and J.A. McCleverty,** *"Comprehensive Coordination Chemistry"* eds.Pergamon.

ix. **Veera Reddy,** *"Symmetry and Spectroscopy of Molecules"*, New Age International Pvt. Ltd., New Delhi (1999).

x. **G. L. Miessler and D. A. Tarr,** "*Inorganic Chemistry"*, 2nd Edn.(1999), Prentice Hall International Inc., London.

Paper -2

CHY-802: Organic Chemistry

Paper Type: Theory Total Hours: 60

Paper type: Core *Total Credits: 4*

Objective:

on completion of this course students will be able to apply the concepts of bonding , aromaticity, stereochemistry, reaction mechanism and different types of stereochemical reactions.

Course Outcomes:

After successful completion of this course, students will be able:

CO1: Explain methods of preparation and applications of organometallic reagents like organo lithium, organo copper, organosilicon, organoborane reagents in organic synthesis.

CO2 : Dicuss the reagents used in reactions like Carbonyl methylenation, carbene insertion and C-H activation.

CO3: Dicuss the reagents used in reactions like Carbonyl methylenation, carbene insertion and C-H activation.

CO4: Discuss Ring formation reactions, ring opening & closing, metathesis, 1,3 dipolar cycloaddition reaction .

CO5: Discuss new synthetic reactions involving c-c coupling reaction, c=c formation reaction, multi component reactions.

CO6: Explain order of events, one bond and two bond C-C and C-X disconnection and control in carbonyl condensation with examples.

Unit-1: Aliphatic Nucleophilic substitution: The S_N2, S_N1, mixed S_N2 and S_N1, and SET **12**mechanism, the neighboring group mechanism, neighboring group participation by σ and Π bonds,anchimeric assistance, classical and non-classical carbocations, phenonium ions, norbornyl system, commoncarbocation rearrangements, application of NMR spectroscopy in the detection of carbocations, the Sn^i mechanism, nucleophilic substitution at an allylic, aliphatic trigonal and vinylic carbon, reactivity effects of substrate structure, attacking nucleophile, leaving group and reactionmedium, phase transfer catalysis and ultrasound, ambident nucleophile, regioselectivity.

Unit-2: Aliphatic Electrophilic substitution: Biomolecular mechanism-SE^2 and SE^1, The SE^i**5** mechanism, electrophilic substitution accompanied by double bond shifts, effect of substrates, leaving group and solvent polarity on the reactivity.

Unit-3: Aromatic Electrophilic substitution: The arenium ion mechanism, orientation and **6** reactivity, energy profile diagrams, the ortho/para ratio, ipso attack, orientation in other ring systems, quantitative treatment of reactivity in substrate and electrophiles, diazonium coupling, vilsmeir reaction, Gatterman Koch reaction.

Unit-4: Aromatic Nucleophilic substitution: The S_NAr, S_N1, benzyne and $S_{RN}1$ mechanisms, **5** reactivity-effect of substrate structure, leaving group and attacking nucleophile, the Von Richter, Sommlet-Houser and Smiles rearrangements.

Unit-5: Free radical reactions: Types of free radical reactions, free radical substitution mechanism,**8**mechanism at an aromatic substrate, neighboring assistance, reactivity for aliphatic and aromaticsubstrates at a bridgehead, reactivity in the attacking radicals, theeffect of solvents on reactivity. allylic halogenation (NBS), oxidation of aldehydes to carboxylic acids, auto- oxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salts, Sandmeyer reaction, free radical rearrangement, Hunsdicker reaction.

Unit-6: Addition to Carbon-Carbon multiple bonds: Mechanistic and stereo chemical aspects of**7** addition reactions involving electrophiles, nucleophiles and free radicals, regio- and chemo selectivity, orientation and reactivity, addition to cyclopropane ring, hydrogenation of double and triple bonds, hydrogenation of aromatic rings, hydroboration, Michael reaction, sharpless asymmetric epoxidation.

Unit-7: Addition to Carbon – Hetero multiple bonds: Mechanism of metal hydride reduction of **12** saturated and unsaturated carbonyl compounds, acids, esters and nitriles, addition of Grignard reagents, organozinc and organolithium reagents to carbonyl and unsaturated carbonyl compounds, Wittig reaction, mechanism of condensation involving enolates- aldol, knovenagel,Claisen, Mannich, benzoin, Perkin and Stobbe Reactions. Hydrolysis of esters and amides, ammonolysis of esters.

Unit-8: Elimination Reactions: The E^2, E^1 and E^1cb mechanisms and their spectrum, orientation **5** of the double bond, reactivity - effects of substrate structures, attacking base, the leaving group and the medium, mechanism and orientation in pyrolytic elimination.

Books Recommended

i. **Jerry March,** *"Advanced Organic Chemistry-Reactions, Mechanism and Structure"*, John Wiley.

ii. **F. A. Carey and R. J. Sundberg,** *"Advanced Organic Chemistry"*, Plenum.

iii. **Peter Sykes,** *"A Guide Book to Mechanism in Organic Chemistry"*, Longman.

iv. **C. K. Ingold,***"Structure and Mechanism in Organic Chemistry"*, Cornell University Press.

v. **R. T. Morrison and R. N. Boyd,** *"Organic Chemistry",*Prentice-Hall.

vi. **H. O. House,***"Modern Organic Reactions",* Benjamin.

vii. **R. O. C. Noman and J. M. Coxon,***"Principles of Organic Synthesis",* Blackie Academic & Professional.

viii. **S. M. Mukherjee and S.P. Singh,** "*Reaction Mechanism in Organic Chemistry"*, Ist Edition(1990),Macmillan India Ltd., New Delhi.

ix. **D. Nasipuri,***"Stereochemistry of Organic Compounds",* New Age International,

x. **P.S. Kalsi,***"Stereochemistry of Organic Compounds",* New Age International.

xi. **T.H. Lowry and K.S. Richardson,** "*Mechanism and Theory in Organic Chemistry"*, 3rd Edition (1998), Addison – Wesley Longman Inc. (IS Edition).

xii. **G. S. Zweifel and M. H. Nantz,***"Modern Organic Synthesis",* (2007), Freeman and Company, New York.

xiii. **M. S. Singh,***"Advanced Organic Chemistry: Reactions and Mechanism"*: Pearson Education (Singapore) Pte. Ltd.

Paper -3

CHY-803: Physical Chemistry

Paper Type: Theory Total Hours: 60

Paper type: Core Total Credits: 4

Objective:

The objective of this course is to acquaint the students with the knowledge of various concepts and principles related to physical chemistry and electrochemistry. Designed as per current syllabus NEP-2022 Guidelines and recent research trends in the topic.

Course Outcomes:

After successful completion of this course, students will be able:

CO1: Students will understand the fundamentals of Chemical dynamics, Oscillatory reaction and method of fast reactions.

CO2: Students will be able to understand the surface chemistry like adsorption and colloidal chemistry and the chemical reactions.

CO3: To understand the concept of macromolecules and determination of molecular weight of the polymer and their application.

CO4: Students come to know about applied electrochemistry and electrochemical catalysis reactions. Butler volmer equation, Tafel plot and Ilkovic equation is necessary for the electrochemical concept.

CO5: This course will equip the students with the necessary detailed chemical knowledge concerning the chemistry of macromolecules.

CO6: Students will be skilled in problem solving, critical thinking and analytical reasoning as applied to scientific problems.

Unit-1: Chemical dynamics: **20**

Methods of determining rate laws, collision theory of reaction rates, steric factor, activated complex theory, rhenius equation and the activated complex theory, ionic reactions, kinetic salt effects, steady state kinetics, netic and thermodynamic control of reactions, treatment of unimolecular reactions. Dynamic chain (hydrogen-bromine reaction, pyrolysis of acetaldehyde, decomposition of ethane), photochemical (hydrogen-omine and hydrogen–chloride reactions) and oscillatory reactions (Belousov- Zhabotinsky reaction),

ɔmogeneous catalysis, kinetics of enzyme reaction, general features of fast reactions, study of fast reactionsby ɔw method, relaxation method, flash photolysis and the nuclear magnetic resonance method. Dynamics of olecular motions, probing the transition state, dynamics of barrierless chemical reactions in solution, dynamics of ıimolecular reactions (Lindmann- Hinshelwood and Rice-Ramsperger- Kassel-Marcus [RRKM], theories of ıimolecular reactions)

Unit-2: .Surface Chemistry: 20

1.Adsorption: Surface tension, capillary action, pressure difference across curved surface (Laplace equation), vapour pressure of droplets (Kelvin equation), Gibbs adsorption isotherm, estimation of surface area (BET equation), surface films on liquids (electro-kinetic phenomenon), and catalytic activity surfaces.

2. Micelles: Surface active agents, classification of surface active agents, micellization, Hydrophobic interaction, Critical Micellar Concentration (CMC), Factors affecting the CMC of Surfactants, Counter Ion Binding to Micelles, Thermodynamics of Micellization-Phase Separation and Mass Action Models, Solubilization, Micro Emulsion, Reverse micelles.

3.Macromolecules: Polymer-Definition, Types of Polymers, Electrically conducting, Fire Resistant, Liquid Crystal Polymers, Kinetics of Polymerization, Mechanism of Polymerization, Molecular Mass, Number and Mass Average Molecular Mass, Molecular Mass Determination (Osmometry, viscometry, Diffusion and light scattering methods),Sedimentation, Chain Configuration of Macromolecules, Calculation of Average Dimensions of Various Chain Structures.

Unit-3: Electrochemistry: Electrochemistry of solutions, Debye-Huckel-Onsager electro treatment **15**

and its extension, ion solvent intractions, Debye-Huckel- Jerum mode, Thermodynamicsof electrified interface equations, Derivation of electro-capillarity, Lippmann equations(surface excess), Methods of determination, structure of electrified interfaces,Guoy –Chapman, Stern, Graham- Devanathan-mottwatts, Tobin, Bockris, Devanathanmodels, over potentials, exchange current density, derivation of Butler-Volmer equation, Tafel plot, quantum aspects of charge transfer at electrodes-solution interfaces,quantization of charge transfer, tunneling, semiconductor interfaces-theory of double layer at semiconductor, electrolyte solutioninterfaces, structure of double layer interfaces, effect of light at semiconductor solution interface.

3. Electrocatalysis – Influence of various parameters, hydrogen **5** electrode. bioelectrochemistry, threshold membrane phenomena, Nernst-Plankequation, Hodges- polarography theory, Ilkovic equation, half wave potential and its significance, introduction to corrosion, homogenous theory, forms of

corrosion, monitoring and prevention methods for corrosion

Books Recommended

i.**P.W. Atkins,***"Physical Chemistry"*, ELBS.

ii.**A.K. Chandra,** *"Introduction to Quantum Chemistry",* Tata McGraw Hill,

iii.**K. J. Laidler,***"Chemical Kinetics"*, Mcgraw-Hill,

iv. **J. Rajaraman and J. Kuriacose,** *"Kinetics and Mechanism of Chemical Transformations",* McMillan

v.**Morol,***"Micelles, Theoretical and Applied Aspects",*Plenum

vi.**J.O.M. Bockris and A.K.N. Reddy,** *"Modern Electrochemistry"* Vol. I and Vol. II, Plenum.

Press, New York (1998).

vii.**V.R. Gowankar, N.V. Vishwanathan and J. Sridhar,**"*Introduction to Polymer Science*", Wiley Eastem.

viii. **J.O'M. Bockris and A. K. N. Reddy,***"Modern Electrochemistry"*,Vol. 2 A & B, 2nd Edition,Plenum Press, New York (1998).

ix. **A.J. Bard and L.R. Faulkner,***"Electrochemical Methods: Fundamentals and Applications"*, 2nd Edition (2001), John Wiley & Sons, New York.

x. **Y. Moroi,***"Micelles: Theoretical and Applied Aspects",*Plenum Press, New York (1992).

xi **F.W. Billmayer Jr.,** *"Text Book of Polymer Science",* 3rd Edition (1984), Wiley-Inter Science, New York.

xii. **I. Prigogine,***"Introduction of Thermodynamics of irreversible Processes"*.

Paper -4

CHY-804: Spectroscopy

Paper Type: Theory Total Hours: 60

Paper type: Core Total Credits: 4

Objective:

The objective of this course is to acquaint the students with the knowledge of various concept spectroscopy. Designed as per current syllabus NEP-2022 Guidelines and recent research trends in the topic.

Course Outcomes:

After successful completion of this course, students will be able:

CO1: Classification of Microwave Spectroscopy and their implication on electron spin interaction.

CO2: Describe the principles of spectroscopic methods such as NMR, IR and UV-Vis.

CO3: Demonstrate a good understanding of the electromagnetic spectrum and how this can be applied to the study of chemical molecules.

CO4: Instrumentation and Application of Nuclear Magnetic Resonance Spectroscopy

CO5: This course will equip the students with the necessary detailed **X-ray diffraction:** Bragg condition, miller indices, laue method, Bragg method

CO6: Students will be skilled in problem solving, critical thinking and analytical reasoning as applied to scientific problems.

Unit-1: Microwave Spectroscopy: classification of molecules, molecular requirement for **4**

rotational spectra, the molecule as a rigid rotor, non-rigid rotor, effect of isotopic substitution on the transition

frequencies, intensities, stark effect, nuclear and electron spin interaction and effect of external field, application.

Unit-2: Vibrational Spectroscopy: 12

A. Infrared Spectroscopy: linear harmonic oscillator, features of vibrational- rotational spectra, vibrational energies of diatomic molecules, zero point energy, frequency, force constant and bond strengths, molecules as an harmonic oscillator, morse potential energy diagram, the interaction of rotations and vibrations, molecules as vibratingrotator: fine structure of infra-red bands, P, Q and R branches, breakdown of oppenheimer approximation, vibration of polyatomic molecules, selection rules, normal modes ofvibration, group frequencies, overtones, Thermal distribution of vibrational & rotational levels, factors affecting the band positions and intensities, analysis and application of infrared spectroscopy.

B. **Raman Spectroscopy:** Classical and Quantum theories of Raman effect, pure rotational, vibrational and vibrational-rotational Raman spectra, coherent anti stokes and stokes lines, selection rules, mutual exclusion principle, resonance Raman spectroscopy, infrared *vs.* Raman spectroscopy.

Unit-3: Electronic Spectroscopy: 12

C. **Atomic Spectroscopy:** structure of atoms, atomic quantum number, energies ofatomic orbital, electronic angular momentum, vector representation of momenta and vector coupling, spectra of hydrogenatom and alkali metal atoms.

D. **Molecular Spectroscopy:** Energy levels, molecular orbitals, vibronic transitions, vibrationalprogressions and geometry of the excited states, Frank Condon principle, electronic spectra of polyatomic molecules, predissociation, emission spectra,radioactive and non-radioactive decay, internal conversion, spectra of transition metal complexes, charge transfer spectra.

Unit-4: Magnetic Resonance Spectroscopy: 20

E. **Nuclear Magnetic Resonance Spectroscopy:** Nuclear spin, interaction between spin and a magnetic field, nuclear resonance, shielding of magnetic nuclei, chemical shift and its measurements, factors influencing chemical shift, de-shielding, spin- spin interactions, factors influencing coupling constant 'J', classification to AX, A_2, AMX, ABC etc, spin decoupling, basic idea about instrument, NMR studies of nucleiother than proton-^{13}C, ^{19}F and ^{31}P, FTNMR, advantages of FTNMR, useof NMR in medical diagnostics.

F. **Nuclear Quadrupole Resonance Spectroscopy:** Quadrupole nuclei, quadrupole moments, electric field gradient, coupling constant, splitting, applications.

Unit-5: X-ray diffraction: Bragg condition, miller indices, laue method, Bragg method, Debye-**12**
Scherrer method of X-ray structural analysis of crystals, indexreflections, identification of unit cells from systematic absences in diffraction pattern, structure of simple lattices and X-ray intensities, structure factor andits relation to intensity and electron density, phase problem, description of the procedure for an X-ray structure analysis, absolute configuration of molecules, Ramchandran diagram.

Books Recommended

i. **R.S. Drago,** *"Physical Methods for Chemistry"*, Saunders Company.

ii. **E.A.V. Ebsworth, D.W.H. Rankin and S. Cradock,** *"Structural Methods in Inorganic Chemistry",* ELBS

iii. **K. Nakamoto,** *"Infrared and Raman Spectra: Inorganic and Coordination Compounds"*, Wiley.

iv. **F.A. Cotton,** *"Progress in Inorganic Chemistry"*vol., 8. ed.,and**S.J. Lippard,** vol., 15, ed. Wiley.

iv. **R.L. Carlin,** *"Transition Metal Chemistry*", vol. 3, Dekker.

v. **A.P.B. Lever,** *"Inorganic Electronic Spectroscopy",* Elsevier 6.

vi. **R.V. Parish**, *"NMR, NOR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry"*,Ellis Horwood.

vii.**M.L Martin, J.J. Delpeuch and G.J. Martin,***"Practical NMR Spectroscopy"*, Heyden.

viii.**R. M. Silverstein, G. C. Bassler and T. C. Mornill,** *"Spectrometric Identification of Organic Compounds",* John Wiley.

ix. **R. J. Abraham, J. Fisher and P. Loftus,** *"Introduction to NMR Spectroscopy"*, Wiley

x. **J. R. Dyer,** *"Application of Spectroscopy of Organic Compounds"*, Prentice Hall,

xi. **D. H. Williams,***"Spectroscopic Methods in Organic Chemistry*", 1. Fleming, Tata McGraw-Hill.

Practical

Semester -VIII

CHY - 805: Practical (Inorganic, Organic, & Physical Chemistry)

Paper Type: Practical — Total Hours: 270

Paper type: Core — Total Credits: 4

Objective:

Impart training in operating different instruments used in the analysis of various chemical constituents.

Course Outcomes:

After successful completion of this course, students will be able:

CO1: Separation and determination of two metal ions Cu-Ni, Ni-Zn, Cu-Fe etc. involving volumetric and gravimetric methods

CO2: Determination of phase equillibria and their determination of congruent composition and temperature of a binary system.

CO3: Determine the distribution coefficient of iodine in different solvents.

CO4: Preparation of different name reactions.

1. Inorganic Chemistry

Qualitative and Quantitative Analysis:

Separation and determination of two metal ions Cu-Ni, Ni-Zn, Cu-Fe etc. involving volumetric and gravimetric methods

2.Organic Chemistry

A.Organic Synthesis:

i. Acetylation: Acetylation of cholesterol and separation of cholesteryl acetate bycolumn chromatography

ii. Oxidation: Adipic acid by chromic acid oxidation of cyclohexanol

iii. Grignard reaction: Synthesis of triphenylmethanol from benzoic acid

iv. Aldol condensation: Dibenzal acetone from benzaldehyde

v. Sandmeyer reaction: p-Chlorotoluene from p-toluidine

vi. Acetoacetic ester Condensation: Synthesis of ethyl-n-butylacetoacetate by A.E.E. condensation.

vii. Cannizzaro reaction: 4-Chlorobenzaldehyde as substrate

viii. Friedel Crafts Reaction: ß-Benzoyl propionic acid from succinic anhydride and benzene

ix. Aromatic electrophilic sustitutions: Synthesis of p-nitroaniline and p- bromoaniline**.**

The Products may be characterized by Spectral Techniques

3. Physical Chemistry

A. Phase Equilibria:

i. Determination of congruent composition and temperature of a binary system (e.g. diphenylamine-benzophenone system)

ii. Determination of glass transition temperature of a given salt (e.g., $CaCl_2$)conductometrically.

iii. To construct the phase diagram for three component system (e.g. chloroform-acetic acid-water).

B.Solutions:

i. Determination of molecular weight of non-volatile and non- electrolyte/electrolyte by cryoscopic method and to determine the activity coefficient of an electrolyte.

ii. Determination of the degree of dissociation of weak electrolyte and to study the deviation from ideal behaviour that occurs with a strong electrolyte.

Books Recommended

i. **J. Derek Woollins,** *"Inorganic Experiments"*, VCH.

ii. **Z. Szafran, R. M. Pike and M. M. Singh,** *"Microscale Inorganic Chemistry"*, Wiley.

iii. **G. Marr and B. W. Rockett,** *"Practical Inorganic Chemistry"*, Van Nostrand.

iv. **J. Bassett. R. C. Denney, G. H.Jeffery and J. Mendham,** *"Vogel's Textbook of Quantitative Analysis, revised"*ELBS.

v. **W. L. Jolly,** *"Synthesis and Characterization of Inorganic Compounds"*, Prentice Hall.

vi. **R. L. Shriner and D. Y. Curtin,** *"The Systematic Identification of Organic Compounds*".

vii. **N. D. Cheronis, J. B. Entrikin and E. M. Hodnett,** *"Semimicro Qualitative Organic Analysis"*

viii. **M. P. Doyle and W. S. Mungall,** *"Experimental Organic Chemistry"*.

ix. **P. J. Hill,** *"Small Scale Organic Preparations"*.

x. **A. M. James and F, E. Prichard,** *"Practical Physical Chemistry"*, Longman.

xi. **B. P. Levitt,** *"Findley's Practical Physical Chemistry"*, Longman.

xii. **R.C. Das and B. Behera,** *"Experimental Physical Chemistry"*, Tata McGrawHill.

Marks Distriution	**Max. Marks**
i. Inorganic Exercise	20
ii. Organic Exercise	20
iii. Physical Exercise	20
iv. Record	8
v. Viva- voce	7
	Total- 75

SEMESTER – IX

Paper -1

CHY - 901: Application of Spectroscopy

Paper Type: Theory Total Hours: 60

Paper type: Core *Total Credits: 4*

Objective:

The objective of the core paper Electronic spectra and magnetic properties of transition metal complexes focuses on charge transfer spectra, spectroscopic method of assignment of absolute configuration.

Course Outcomes:

After successful completion of this course, students will be able:

CO1: Symmetry and shape AB2, AB3,AB4,AB5 and AB6 mode of vibration spectra .

CO2: Study Electron Spin Resonance Spectroscopy

CO3: Study Mossobauer Spectroscopy

CO4: Study important concepts of UV-Visible Spectroscopy and its role in structure elucidation of organic compounds

CO5: Study important concepts of Infrared Spectroscopy and its role in structure elucidation of organic compounds

CO6: Study important concepts of 1H NMR and 13C NMR spectroscopy and its role in structure elucidation of organic compounds

CO7: Study important concepts of Mass spectrometry and its role in structure elucidation of organic compounds.

Unit-1: Inorganic Chemistry

A. Vibrational spectroscopy: Symmetry and shapes of AB_2, AB_3, AB_4, AB_5 and AB_6, Mode of bonding of ambidentate ligands, ethylenediamine and diketonato complexes, Application ofresonance Raman spectroscopy particularly for the study of active sites of metalloproteins. **5**

B. Electron Spin Resonance Spectroscopy: 7

Hyperfine coupling, spin polarization for atoms and transition metal ions, spin-orbit coupling and significance of g-tensors,application to transition metal complexes (having one unpaired electron) including and $[BH]^{-}$.biological systems and to inorganic free radicals such as PH_4, F

C. Nuclear Magnetic resona[2]nce of P[3]aramagnetic substances in solution: 7

Thecontact and pseudo contact shifts, factors affecting nuclear relaxation, someapplications including biochemical systems, an overview of NMR of metal nuclides with emphasis on ^{195}Pt and ^{119}Sn NMR.

D. Mossbauer Spectroscopy: 6

Basic principles, spectral parameters and spectrum display, application of the technique to the studies of (1) bonding and structures of Fe^{2+} and Fe^{3+} compounds including those of intermediate spin, (2) Sn^{+2} and Sn^{+4} compounds- nature of M-L bond, coordination number, structure and (3) detection of oxidation state and inequivalent MB atoms.

Unit-2: Organic Chemistry

A. Ultraviolet and Visible Spectroscopy: Various electronic transitions (185-800 nm), **3**Beer-Lambert law, effect of solvent on electronic transitions, ultraviolet bands forcarbonyl compounds, unsaturated carbonyl compounds, dienes, conjugated polyenes,Fisher-Woodward rules for conjugated dienes and carbonyl compounds, ultraviolet spectra of aromatic and heterocyclic compounds, steric effects in biphenyls.

B. Infrared Spectroscopy: instrumentation and sample handling,Characteristic vibrational **5**frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols and amines, detailed study of vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters, amides, acids, anhydrides, lactones, lactams and conjugated carbonyl compounds). Effect of hydrogen bonding and solvent effect on vibrational frequencies, overtones, combination bands and Fermi resonance, FTIR, IR of gaseous, solids and polymeric materials.

C. Optical rotatory dispersion and Circular dichroism: **3**

Definition, deduction of absolute configuration, octant rule for ketones.

D. Nuclear Magnetic resonance spectroscopy: General introduction and definition, **10**

chemical shift, spin-spin interaction, shielding mechanism, mechanism, mechanism of measurement, chemical shift values and correlation for protons bonded to carbon (aliphatic, olefinic, aldehydic and aromatic) and other nuclei (alcohols, phenols, enols, carboxylic acids, amines, amides &mercapto), chemical exchange, effect of deuteration, complex spin-spin interaction between two, three, four and five nuclei (first order spectra), virtual coupling, stereochemistry, hindered rotation, Karplus curve-variation of coupling constant with dihedral angle, simplification of complex spectra-nuclear magnetic double

resonance, contact shift reagents, solvents effects, Fourier transform technique, nuclear overhouser effect, resonance of other nuclei-F, P.

E. ^{13}C NMR Spectroscopy: 5

General considerations, chemical shift (aliphatic, olefinic,alkyne, aromatic, heteroaromatic and carbonyl carbon), coupling constants, Two dimension NMR Spectroscopy – COSY, NOESY, DEPT, INEPT, APT and INADEQUATE techniques

F. Mass Spectroscopy: 8

Introduction, ion production-EI, CI, FD and FAB,factors affecting fragmentation, ion analysis, ion abundance, mass spectral fragmentation of organic compounds, common functional groups, molecular ion peak, metastable peak, McLafferty rearrangement, nitrogen rule, high resolution mass spectrometry, examples of mass spectralfragmentation of organic compounds with respect to their structure determination.

Books Recommended

i. **K. Nakamoto,** *"Infrared and Raman Spectra: Inorganic and Coordination Compounds",* Wiley.

ii. **F.A. Cotton,** *"Progress in Inorganic Chemistry"*vol., 8. ed., and **S.J. Lippard,**vol., 15, ed. Wiley.

iii. **E.A.V. Ebsworth, D.W.H. Rankin and S. Cradock,** *"Structural Methods in Inorganic Chemistry",*ELBS.

iv. **N.N. Greenwood and T. C. Gibb,** *"Mossbauer Spectroscopy"*.

v. **R.S. Drago,** *"Physical Methods for Chemistry"*, Saunders Company.

vi. **P.S. Kalsi***"Spectroscopy of Organic Compounds*".

vii. **Colin N. Banwel***"Fundamentals of Molecular Spectroscopy"*Fifth Ed., McGraw Hill.

viii. **A.P.B. Lever,** *"Inorganic Electronic Spectroscopy"*, Elsevier. 6.

ix. **M.L Martin, J.J. Delpeuch and G.J. Martin,** *"Practical NMR Spectroscopy",*Heyden.

x. **R. J. Abraham, J. Fisher and P. Loftus,** *"Introduction to NMR Spectroscopy"*, Wiley

xi. **R.V. Parish,** *"NMR, NOR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry",* Ellis Horwood.

Additional References

1.**John R. Dyer,**"*Application of Absorption Spectroscopy of Organic Compounds",* Prentice Hall, New Delhi (1978).

2. **R.M. Silverstein and F.X. Webster,** *"Spectroscopic Identification of Organic Compounds"*, 6th Edition (2003) John Wiley, New York.

3. **D.H. Williams and I.F. Fleming,**"*Spectroscopic Methods in Organic Chemistry"*, 4th Edition(1988), Tata-McGraw Hill, New Delhi.

Paper -2

CHY - 902: BIOCHEMISTRY

Paper Type: Theory Total Hours: 60

Paper type: Core *Total Credits: 4*

Objective:

The objective of this course is to acquaint the students with the knowledge of various concepts and principles related to physical chemistry and electrochemistry. Designed as per current syllabus NEP-2022 Guidelines and recent research trends in the topic.

Course Outcomes:

After successful completion of this course, students will be able:

CO1: Heme protein and oxygen uptake, structure and function of haemoglobin, myoglobin and hemerythrin, model synthetic complexes of iron, copper and cobalt.
Na+ /K+ pump is Na+ /K+ ATPASE and is found to maintain both magnitude and direction of transmembrane concentration gradients of these ions. Haemoglobin, myoglovin and haemerythrin play important part in the transportation of oxygen.

CO2: Metal compounds are closely related to the life process. Among these compounds are chlorophyll ,numerous haematin enzymes, metal activated enzymes, vitamin B12 and those vital but poorly understood complexes which play an important role in the metabolism of the metal ions.

CO3: Bioenergetics or biochemical thermodynamics is the study of energy G, is the useful energy alsoΔchanges in biochemical reactions. Free energy, known as the chemical potential. In the living cells, the principal high energy intermediate or carrier compound is ATP.

Unit-1: Metal ions in biological systems: Essential and trace metals. **2**

1. Na+/k+ Pump: Role of metals ions in biological processes, **3**

Unit-2: Bioenergetic and ATP Cycle: **6**

DNA polymerization, glucose storage, metalcomplexes in transmission of energy, chlorophylls, photosystem I and photosystem II in cleavage of water, model systems.

Unit-3: Transport and storage of Dioxygen: Heme protein and oxygen uptake, structure and **8**

function of hemoglobin, myoglobin, hemocyanins and hemerythrin, model synthetic complexes of iron, cobalt and copper

Unit-4: Electron Transfer in biology: **6**

Structure and function of metalloproteins in electron transport processes-cytochromes and ion-sulphur proteins, synthetic models.

2. Enzymes: **6**

Introduction and historical perspective, chemical and biological catalysis, remarkable properties of enzymes like catalytic power, specificity and regulation, nomenclature and classification, extraction and purification. Fischer;s lock and key and Koshland's induced fit hypothesis, concept and identification of active site by the use of inhibitors, affinity labeling and enzyme modification by site – directed mutagenesis. Enzyme kinetics, michaelis-menten and lineweaver-burk plots, reversible and irreversible inhibition.

Unit-5: Mechanism of enzyme action:

6Transport state theory, orientation and steric effect, acid-dase catalysis, covalent catalysis, strain or distortion, examples of some typical enzyme mechanisms for chymotrypsin, ribonuclease, Lysozyme and carboxypeptidase A.

Unit-6: Kinds of reactions catalysed by enzymes: Nucleophilic displacement on a**6**

phosphorus atom, multiple displacement reactions and the coupling of ATP cleavage to endergonic processes, transfer of sulphate, addition and elimination reactions, enolic intermediates in isomerization reactions, -cleavage and condensation, some isomerization and rearrangement reactions, Enzyme catalysed carboxylation and decarboxylation.

Unit-7: Co-Enzyme Chemistry: Cofactors as derived from Vitamins, coenzymes, prosthetic**4**

groups, apoenzymes, structure and biological functions of coenzyme A, thiamine pyrophosphate, pyridoxal phosphate, NAD^+, $NADP^+$, FMN, FAD, lipoic acid, vitamin B12, mechanism of reactions catalysed by the above cofactors.

Unit-8: Enzyme models: Host guest chemistry, chiral recognition and catalysis, molecular**4**

recognition, molecular asymmetry and prochirality, biomimetic chemistry, crown ethers, cryptates, cyclodextrins, cyclodextrin-based enzyme models, calixarenes, ionophores, micelles, synthetic enzymes or synzymes.

Unit-9: Biological cell and its constituents: Biological cell, structure and functions of**2**

proteins, enzymes, DNA and RNA in living systems, Helix coil transition.

3. Bioenergetics: Standard free energy change in biochemical reactions, exergonic,**3**

endergonic, hydrolysis of ATP, synthesis of ATP from ADP.

4. Thermodynamics of biopolymer solutions: Thermodynamics of biopolymer solutions, osmotic pressure, membrane equilibrium, muscular contraction and energy generation in mechanochemical system. **4**

Diffraction methods: **3**

Light scattering, low angle X-ray scattering, X-ray diffraction and photo correlation spectroscopy, ORD

Books Recommended

i. **S.J. Lippard and J.M. Berg,** *"Principles of Bioinorganic Chemistry"*, University Science Books.

ii. **T.A. Brawn,** *"Biochemistry".*

iii. **David L. Nelson and Michael M. Cox,** *"Lehninger Principles of Biochemistry".*

iv. **Trevor Palmer Philip Bonner**, *"Understanding Enzymes",* Prentice Hall.

v. **I. Bertini, H.B. Gray, S.J. Lippard and J.S. Valentine,** *"BioinorganicChemistry",*University ScienceBooks.

vi. **G.L. Eichhorn,** *"Inorganic Biochemistry",* vols I and II. Ed, Elsevier.

vii. **J.J. Lippard,** *"Progress in Inorganic Chemistry"* Vols 18 and 38 ed. Wiley.

viii. **M. N. Hughes,** "*Inorganic Chemistry of Biological Processes*", 2nd Ed.(1981), John-Wiley & Sons, New York.

ix. **S. J. Lippard and J. M. Berg,** "*Principles of Bioinorganic Chemistry*", University Science Books, (1994).

x. **W. Kaim and B. Schwederski,** "*Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, An Introduction and Guide*", Wiley, New York (1995).

xi. **I. Bertini, H. B. Grey, S. J. Lippard and J. S. Valentine,** "*Bioinorganic Chemistry*", Viva Books Pvt. Ltd., New Delhi (1998).

xii. **Ed. Collin J Suckling,** *"Enzyme Chemistry: Impact and Applications",* Chapman and Hall.

xiii. **Hermann Dugas and C. Penny,** *"Bioorganic Chemistry: A Chemical Approach to Enzyme Action"*, Springer Verlag.

Paper -3

CHY 9031: Analytical techniques

Paper Type: Theory Total Hours: 60

Paper Type: Elective Paper-I Total Credits: 4

Objective:

The primary objective of this course is to acquire basic concepts, principles, instrumentations and techniques of modern analytical techniques that would empower students with an analytical mind set and the abilities to solve diverse analytical problems in an efficient and quantitative way that conveys the importance of accuracy and precision of the analytical results.

Course Outcomes:

After successful completion of this course, students will be able:

CO1: Students will be able to define what makes a measurement accurate or inaccurate.

CO2: Upon completion of this lab, the student will be able to: Determine the molar concentration of a solution of an acid or base using data obtained from titration.

CO3: Upon completion of this lab, you have an overview of industrial methods for ion exchange and liquid -liquid extraction and examples form radio chemical separation processes.

CO4: After this lesson, students will be able to, Define chromatography, demonstrate an understanding of the process of chromatography and describe the steps involved in a chromatography investigation.

CO5: Understanding various experimental measurement techniques involved in the field of thermal analysis and understanding the concept of measured data analysis and data acquisition technique.

Unit-1: Significant figures; Determinate and Indeterminate errors, absolute and relative errors, **08**
error curves, minimization of errors; precision and accuracy, determination of accuracy; mean, Median and mode; standard deviation.

Unit-2: Principles, instrumentation and applications of the following techniques: **15**
i. Complexometric, Chelatometric and Non-aqueous titration.
ii. Potentiometric and Conductometric Titrations.
iii. Polarography and Amperometry
iv. Coulometry and Voltametry (With special reference to cyclic voltametry and Annodic Stripping voltametry).

Unit-3: Principles and applications of solvent extraction and ion exchange resins. **12**

Unit-4: Fundamental principles of chromatography. Principles, instrumentation and applications of column chromatography, paper chromatography, thin layer chromatography, gas chromatography, radial chromatography and HPLC. **15**

Unit-5: Techniques and principles of Thermal Analysis: TGA, DTA and DSC. **10**

Books Recommended

1. D.A. Skoog, F.J. Holler and T.A. Nieman, "Principles of Instrumental Analysis", 5th Edition (1998), Saunders College Publishing, Philadelphia, London.Harcourt Brace & Company, U.S.A.
2. G.W. Ewing, "Instrumental Methods of Chemical Analysis", 5th Edition (1978), McGraw Hill Books Co., New York.
3. R.l. Pecsok, L.D. Shields, T. Cairns and L.C. Mc Williams, "Modern Methods of Chemical Analysis", 2nd Edition (1976), john Wiley, New York.
4. J.H. Kennedy, " Analytical Chemistry: Principles", 2nd Edition (1990), Saunders Holt, London.
5. L. Meites, "Polarographic Techniques", 2nd Edition (1965), John Wiley, New York.
6. J. Heyrovsky and K. Kuta, "Principles of Polarography", 1st Edition (1966), Academic Press, New York.
7. A. J. Bard and L.R. Faulkner, "Electrochemical Methods: Fundamentals and Applications", 2nd Edition (2000), Wiley, New York.

Additional References

1. I.M. Kolthoff and J.J. Lingane, "Polarography", 2nd Edition (1952), Wiley Intersciences, New York.
2. C.W.C. Milner and G. Phillips, "Coulometry in Analytical Chemistry", Pregamon Press, New York (1967).

Paper -3

CHY 9032: Liquid state

Paper Type: Theory Total Hours: 60

Paper Type: Elective Paper-I Total Credits: 4

Objective:

The primary objective of this course is to acquire basic concepts, principles, Liquids state

Course Outcomes:

After successful completion of this course, students will be able:

CO1: Study of general properties of Liquids.

CO2: Theory of liquids.

CO3: Distribution function and related equations.

CO4: Methods for structure determination and computational techniques.

CO5: Supercooled and Ionic liquids.

1. **General Properties of Liquids: 13**

a) Liquids as dense gases, liquids as disordered solids, some thermodynamic relations, internal pressure and its significance in liquids. Equations of state and critical constants. Different types of intermolecular forces in liquids, different potential functions for liquids, additivity of pair potential approximation.

b) A classical partition function for liquids, correspondence principle, configuration configuration properties.

2. **Theory of Liquids:** Theory of liquids, partition function method or model **9**

approach; single cell models, communal energy and entropy, LTD model, significant structure model.

3. **Distribution Function and Related Equations:** Radial distribution function **14**

method, equation of state in terms of RDF. Molecular distribution functions, pair distribution function. Relationship between pair distribution function and pair potential function. The IBG equation, the HNC equation, the PY equation, cluster expansion.

4. **Methods for Structure Determination and Computational Techniques: 12**

Spectroscopic techniques for liquid dynamic, structure studies, Neutron and X- ray scattering spectroscopy.

Computation Techniques-Monte, Carlo and molecular dynamics methods.

5. **Supercooled and Ionic Liquids:** Supercooled and ionic liquids, theories of transport properties; non Arrhenius behaviour of transport properties, Cohen- Tumbull free volume model, configurational entropy model, Macedo-Litovitz hybrid model, glass transition in supercooled liquids. **12**

Books Suggested

i. **P.A. Egelstalf,** *"An Introduction to Liquid State"*, Academic Press.

ii. **A.F.M. Barton,***"The Dynamic Liquid State"*, Longman

iii. **T.L. Hill,** *"Introduction to Statistical Thermodynamics",* Addison Wiley.

iv. **J.A. Pryde,***"The Liquid State"*.

v. **H. Eyring and MS. John,***"Significant Liquid Structures"*.

Paper -3

CHY-9033 : Bioinorganic Supramolecular Chemistry

Paper Type: Theory Total Hours: 60

Paper Type: Elective Paper-I Total Credits: 4

Objective:

The objective of this course is to acquire basic concepts, principles of Bioinorganic and supramolecular chemistry.

Course Outcomes:

After successful completion of this course, students will be able:

CO1: Study Metalloenzymes

CO2: Understand chemistry of Photosynthesis

CO3: Understand transport and storage of dioxygen through different carriers

CO4: Study Electron Transfer in Biology involving metaloproteins and cytochromes

CO5: Biological nitrogen fixation

CO6: Role of Metals in Medicine

CO7: Understand the underlying concepts of Supramolecular Chemistry such as hostguest interactions, molecular recognition host design, templates and self assembly

CO8: Study of Crown ethers Cryptands, Spherands, Podants, expanded porphyrins, guanidinium based receptors, solid state clatharates, zeolites

1. **Metal Storage Transport and Biomineralization:** Ferritin, transferrin, and siderophores **5**

2. **Calcium in Biology:** Calcium in living cells, transport and regulation, molecular aspects of **6** intramolecular processes, extracellular binding proteins.

3. **Metalloenzymes:** Zinc enzymes - carboxypeptidase and carbonic anhydrase. Iron enzymes **20** - catalase, peroxidase and cytochrome P-450. Copper enzymes - superoxide dismutase.

Molybdenum oxatransferase enzymes - xanthine oxidase. Coenzyme vitamin B12

4. Metal-Nucleic Acid Interactions: Metal ions and metal complex interactions. Metal complexes - nucleic acids. **6**

5. Metals in Medicine: Metal deficiency and disease, toxic effects of metals, metals used for diagnosis and chemotherapy with particular reference to anticancer drugs. **5**

6. Supramolecular Chemistry: 12

i. Concepts and language.

ii. Molecular recognition: Molecular receptors for different types of molecules including arisonic substrates, design and synthesis of coreceptor molecules and multiple recognition.

iii. Supramolecular reactivity and catalysis.

iv. Transport processes and carrier design.

v. Supramolecular devices. Supramolecular photochemistry, supramolecular electronic, ionic and switching devices. Some example of self-assembly in supramolecular chemistry

Books Recommended

i. **S.J. Lippard and J.M. Berg,** *"Principles of Bioinorganic Chemistry"*, University Science Books.

ii. **I. Bertini, H.B. Gray, S.J. Lippard and J.S. Valentine,***"Bio-norganic Chemistry*", University Science Books.

iii. **G.L. Eichhom,** *"Inorganic Biochemistry"*, vols I and II. ed., Elsevier.

iv. **J.J. Lippard,***"Progress Inorganic Chemistry",* Vols 18 and 38 ed. Wiley.

v. **J.M. Lehn**, *"Supramolecular Chemistry"*,VCH.

Paper -3

CHY – 9034 Organic Synthesis

Paper Type: Theory Total Hours: 60

Paper Type: Elective Paper-I Total Credits: 4

Objective:

Organic synthesis involves strategies for making compounds from readily available starting materials by one or more steps. The heart of organic synthesis is designing synthetic routes to a molecule.Selectivity is an important consideration when determining a synthetic route to a target molecule. Chemists need to consider both stereoselectivity and chemoselectivity in organic synthesis.Synthetic reactions can be categorized based on whether they involve functional group interconversion or carbon-carbon bond formation.

Course Outcomes:

After successful completion of this course, students will be able:

CO1 Explain methods of preparation and applications of organometallic reagents like organo lithium, organo copper, organosilicon, organoborane reagents in organic synthesis.

CO2 Dicuss the reagents used in reactions like Carbonyl methylenation, carbene insertion and C-H activation.

CO3 Discuss different types of reagents used for oxidation and reduction reactions.

CO4 Make use of various rearrangement reactions for synthesis of various compounds.

A. Organometallic Reagents: Principle, preparations, properties and applications of the **30**

following inorganic synthesis with mechanistic details-

i.Group I and II metal organic compounds

ii.Li, Mg, Hg, Cd, Zn and Ce compounds.

iii.Transition metals

iv. Cu, Pd, Ni, Fe, Co, Rh, Cr and Ti compounds.

v. Other elements

vi. S, Si, B and I compounds.

B. Oxidation: 10

Introduction. Different oxidative processes. Hydrocarbons-alkenes, aromatic rings, saturated C-H groups (activated and unactivated). Alcohols, diols, aldehydes, ketones, ketals and carboxyalic acids, Amines,

hydrazines, and sulphides. Oxidations with ruthenium tetraoxide, iodobenzene diacetate and thallium nitrate.

C. Reduction: 10

Introduction. Different reductive processes.

Hydrocarbons- alkanes, alkenes, alkynes and aromatic rings. Carbonyl compounds-aldehydes, ketones, acids and their derivatives. Exposides. Nitro, nitroso, azo and oxime groups. Hydrogenolysis.

D. Rearrangements: 10

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

Books Recommended

i. **H.O.House and W. A. Benjamin,** *"Modem Synthetic Reactions"*.

ii. **W. Camuthers,** *"Some Modern Methods of Organic Synthesis"*, Cambridge Univ. Press.

iii. **J. March,***"Advanced Organic Chemistry, Reactions Mechanisms and Structure",* John Wiley.

iv. **R. O. C. Norman and J. M. Coxon,***"Principles of Organic Synthesis"*, Blackie Academic &Professional.

v. **F. A. Carey and R. J. Sundberg,***"Advanced Organic Chemistry Part B*". Plenum Press.

vi. **Ed. S. Coffey,***"Rodd's Chemistry of Carbon Compounds*", Elsevier.

Paper -4

CHY-9041: Analytical Chemistry

Paper Type: Theory Total Hours: 60

Paper type: Elective paper-II Total Credits: 4

Objective:

The primary objective of this course is to acquire basic concepts, principles, and techniques of modern analytical chemistry that would empower students with an analytical mind set and the abilities to solve diverse analytical problems in an efficient and quantitative way that conveys the importance of accuracy and precision of the analytical results

Course Outcomes:

After successful completion of this course, students will be able:

CO1: To develop an understanding of the range and uses of analytical methods in chemistry.

CO2: To establish an appreciation of the role of chemistry in quantitative analysis.

CO3: To develop an understanding of the broad role of the chemist in measurement and problem solving for analytical tasks.

CO4: To provide an understanding of chemical methods employed for elemental and compound analysis.

CO5:to provide experience in some scientific methods employed in analytical chemistry. 6. to develop some understanding of the professional and safety responsibilities residing in working on chemical analysis.

CO6: Students will be able to design and carry out scientific experiments as well as accurately record and analyze the results of such experiments.

CO7: Students will be proficient in problem solving, critical thinking, and analytical reasoning as applied to scientific problems.

Unit-1: **Introduction:** Role of analytical chemistry. Classification of analytical methods-classical and instrumental. Types of instrumental analysis. Selecting an analytical method. Neatness and cleanliness. Laboratory operations and practices. Analytical balance. Techniques of weighing, errors. Volumetric glassware-cleaning and calibration of glassware. Sample preparations dissolution and decompositions. Gravimetric techniques. Selecting and handling of reagents. Laboratory notebooks. Safety in the analytical laboratory. **12**

Unit-2:Errors and Evaluation: Definition of terms in mean and median. Precision-standard deviation, relative standard deviation. Accuracy-absolute error, relative error. Types of error in experimental data determinate (systematic), indeterminate (or random) and gross. Sources of errors and the effects upon the analytical results. Methods for reporting analytical data. Statistical evaluation of data-indeterminate errors. The uses of statistics **7**

Unit-3:Food Analysis: Moisture, ash, crude protein, fat, crude fibre, carbohydrates, calcium, potassium, sodium and phosphate. Food adulteration-common adulterants in food, contamination of food stuffs. Microscopic examination of foods for adulterants. Pesticide analysis in food products. Extraction and purification of sample. HPLC. Gas chromatography for organophosphates. Thin-layer chromatography for identification of chlorinated pesticides in food products. **12**

Unit-4: Analysis of Water Pollution: Origin of waste water, types, water pollutants and their effects. Sources of water pollution domestic, industrial, agricultural soil and radioactive wastes as sources of pollution. Objectives of analysis-parameter for analysis-colour, turbidity, total solids, conductivity, acidity, alkalinity, hardness, chloride, sulphate, fluoride, silica, phosphates and different forms of nitrogen. Heavy metal pollution-public health significance of cadmium, chromium, copper, lead, zinc, manganese, mercury and arsenic. General survey of instrumental technique for the analysis of heavy metals in aqueous systems. Measurements of DO, BOD and COD. Pesticides as water pollutants and analysis. Water pollution laws and standards. **12**

Unit-5: Analysis of Soil, Fuel, Body Fluids and Drugs:

i. Analysis of soil: moisture, pH, total nitrogen, phosphorus, silica, lime, magnesia, manganese, sulphur and alkali salts.

ii. Fuel analysis: solid, liquid and gas. Ultimate and proximate analysis-heating values grading of coal. Liquid fuels-flash point, aniline point, aclane number and carbon residue. Gaseous fuels-producer gas and water gas-calorific value.

iii. Clinical chemistry: Composition of blood collection and preservation of samples. Clinical analysis. Serum electrolytes, blood glucose, blood urea nitrogen, uric acid, albumin, globulins, barbiturates, acid and alkaline phosphatases. Immunoassay: principles of radio immunoassay (RIA) and applications. The blood gas analysis trace elements in the body.

iv. Drug analysis: Narcotics and dangerous drugs. Classification of drugs. Screening gas and thin-layer chromatography and spectrophotometric measurements.

Books Recommended

i. **G.D. Christian,** *"Analytical Chemistry",* J. Wiley.

ii. **D.A. Skoog, D M. West and F.J. Holler,***"Fundamentals of Analytical Chemistry",* W. B. Saunders.

iii. **J.H. Kennedy,***"Analytical Chemistry-Principles*", W. B. Saunders

iv. **L.G. Harps,** *"Analytical Chemistry-Principles and Techniques",* Prentice Hall.

v. **D.A. Skoog and J.L. Loary,** *"Principles of Instrumental Analysis",* W. B. Saunders.

vi. **R.A. Day, Jr. and A.L. Underwood,** *"Quantitative Analysis"*, Prentice Hall.

vii. **S.M. Khopkar,***"Environmental Solution Analysis"*, Wiley Eastern.

ix. **S M. Khopkar,***"Basic Concepts of Analytical Chemistry"*, Wiley Eastern.

x. **F. Settle,***"Handbook of instrumental Techniques for Analytical Chemistry",* Prentice Hall.

Paper -4

CHY-9042: Organotransition Metal Chemistry

Paper Type: Theory — Total Hours: 60

Paper type: Elective paper-II — Total Credits: 4

Objective:

The objective of the core paper Electronic spectra and magnetic properties of transition metal complexes focuses on charge transfer spectra, spectroscopic method of assignment of absolute configuration.

Course Outcomes:

After successful completion of this course, students will be able:

CO1: Understand alkyls and aryls of transition Metals

CO2: Study compounds of Transition Metal with Carbenes and Carbynes.

CO3: Study Transition Metal π Complexes

CO4: Understand Catalysis involving organometallic compounds

CO5: Study Fluxional organometallic Compounds

1. **Alkyls and Aryls of Transition Metals:** Types, routes of synthesis, stability and decomposition pathways, organocopper in organic synthesis **5**

2. Compounds of Transition Metal-Carbon Multiple Bonds: 12

Alkylidenes, alkylidynes, lowvalent carbenes and carbynes- synthesis, nature of bond, structural characteristics,nucleophilic and electrophilic reactions or the ligands, role in organic synthesis.

3. Transition Metal π –Complexes: 18

Transition metal π-complexes with unsaturated organic molecules, alkenes, alkynes, ailyl, diene, dienyl, arene and trienyl complexes, preparations, properties, nature of bonding and structural features. Important reactions relating to nucleophilic and electrophilic attack on ligands and to organic synthesis

4. Transition Metal Compounds with Bonds to Hydrogen: **3**

Transition metal compoundswith bonds to hydrogen.

5. Homogeneous Catalysis: Stoichiometric reactions for catalysis, homogeneous catalytic **14** hydrogenation, Zeigler-Natta polymerization of olefins, catalytic reactions involving carbon monoxide such as hydrocarbonylation of clefins (oxo reaction), oxopalladation reactions, activation of C-H bond.

6. Fluxional Organometallic Compounds: 8

Fluxionality and dynamic equilibria in compounds such as n olefin, n^{23} allyl and dieny! complexes

Books Recommended

i. **J.P. Colanan, L.S. Heysdus. J.R. Norton and H.G. Finke,** *"Principles and Application of Organotransition Metal Chemistry",*University Science Books.

ii. **R.H. Crabtree,** *"The Organometallic Chemistry of the Transition Metals",* John Wiley

iii. **A.J. Pearson,** *"Motalo-organic Chemistry"*, Wiley.

iv. **F.A. Cotton and G. Wilkinson,***"Advanced Inorganic Chemistry"*, 6th Ed. (1999) John Wiley & Sons, NY.

v. **Ch. Elschenbroich and A. Salzer,** *"Organometallics"*, VCH.

vi. **J.P. Collman, L.S. Hegedus, J.R. Norton and R.G. Finke,***"Principles and Applications of Organotransition metal Chemistry",* Univ. Sci. Books, Mill Valley. California.

iv. **R.C. Mehrotra and A. Singh,** *"Organometallic Chemistry"*, New Age International.

Paper -4

CHY–9043 Natural Products

Paper Type: Theory Total Hours: 60

Paper type: Elective paper-II Total Credits: 4

Objective:

The course provides provide an overview of the field of natural product chemistry. It lays emphasis on classification, nomenclature, structure, biosynthesis, occurrence, analysis and pharmaceutical perspectives.

Course Outcomes:

After successful completion of this course, students will be able:

CO1: provides an overview of the field of natural product chemistry. Gain knowledge about various terpenoids, their stereochemistry, biosynthesis, structural determination, synthesis and medicinal importance.

CO2 : Explains structure, occurrence, biosynthesis, stereochemistry, classification and importance of various alkaloids

CO3: studies the different types of steroids, their occurrence, structure, biosynthesis and properties, as well as important steroid hormones.

CO4: Determines biosynthetic mechanisms, discusses feeding experiments of biosynthetic precursors and secondary metabolites. Explain with examples the acetate-malonate pathway, shikimic acid pathway and mevalonic acid pathway of secondary metabolites.

CO5: Discuss the occurrence, nomenclature, classification, biogenesis and physiological effects of using natural products as starting materials for drugs.

CO6: To conduct independent testing of plant materials and natural products.

1. Terpenoids and Carotenoids: 15

Classification, nomenclature, occurrence, isolation,general methods of structure determination, isoprene rule. Structure determination,stereochemistry, biosynthesis and synthesis of the following representative molecules: Citral, Geraniol, α-Terpeneol, Menthol, Farnesol, Zingiberene, Santonin, Phytol, Abiatic acid and β-Carotene.

2. Alkaloids: 15

Definition, nomenclature and physiological action, occurrence, isolation, generalmethods of structure elucidation, degradatin, classification based on nitrogen heterocyclic ring, role of

alkeloids in plants. Structure, stereochemistry, synthesis and biosynthesis of the following: Ephedrine, (+)- Conviine, Nicotine, Atropine, Quinine and Morphine.

3. Steroids: 15

Occurrence, nomenclature. basic skeleton, Diel's hydrocarbon and stereochemistry.Isolation, structure determination and synthesis of Cholesterol, Bile acids, Androsterone., Testosterone, Estrone, Progestrone, Aldosterone. Biosynthesis of steroids.

4 Plant Pigments: 7

Occurrence, nomenclature and general methods of structuredetermination, isolationand synthesis of Apigenin, Luteoline, Quercetin, Myrectin, Quercetin-3-glucoside, Diadzein, Butein, Aureusin I Cyandin-7-arabinoside, cyanidin, Hirsutidin. Biosynthesis of flavonoids : Acetate pathway and Shikimic acid pathway.

5.Porphyrins: Structure and synthesis of Hemoglobin and Chlorophyl **3**

6 Prostaglandins: 3

Occurrence, nomenclature, classification, biogenesis and physiological effects. Synthesis of PGE_2 and PGF 2'

7 Pyrethroids and Rotenones: 2

Syathesis and reactions of Pyrethroids and Retenones. (For structtJre elucidation, emphasis is to be place on the use of spectral parameters wherever possible).

Books Recommended

1. **Nitya Anand, J.S. Bindra and S. Ranganathan,**"*Art in Organic Synthesis"*, 2nd Edition (1970), Holden Day, San Francisco.
2. **S.W. Pelletier,**"*Chemistry of the Alkaloids"*, Van Nostrand Reinhold Co., New York (1970).
3. **K.W. Bentley,**"*The Alkaloids"*, Vol. I., Interscience Publishers, New York (1957).
4. **I. L. Finar**, "*Organic Chemistry"*, Vol. II, 5th Edition (1975) Reprinted in 1996, ELBS and Longman Ltd, New Delhi
5. **J.W. Apsimon,**"*Total Synthesis of Natural Products",* Vol. 1-6, Wiley-Interscience Publications, New York (Vol. 1, 1973).
6. **J.S. Bindra and R. Bindra** ,"*Creativity in Organic Synthesis",* Academic Press, NY (1975).
7. **J.S. Bindra and R. Bindra,**"*Prostaglandins Synthesis",* Academic Press. Inc., New York, London (1977).
8. **K. C. Nicolaou,**"*Classics in Total Synthesis of Natural Products",* Vol. I (1996) & Vol. II (2003).
9. **J. Clayden, N. Greeves, S. Warren, and P. Wothers,**"*Organic Chemistry, Chapter 30",* Oxford University Press, Oxford (2001).

Paper -4

CHY – 9044 : Advanced Quantum Chemistry

Paper Type: Theory Total Hours: 60

Paper type: Elective paper-II Total Credits: 4

Objective:

Physical chemistry are focused on understanding themacro and microscopic properties. Their discoveries are based on understanding chemical thermodynamics, statistical thermodynamics and quantum chemistry describing their behavior using theories of physics and mathematical computations

Course Outcomes:

After successful completion of this course, students will be able:

CO1: Theoritical and Computational treatment of atoms and molecules, Hartree-Fock Theory.

CO2: Configuration Interaction and MC-SCF.

CO3: Study of Semi-emperical theories.

CO4: Study of Density functional theory.

CO5: Study of Computer experiments.

i. Theoretical and Computational Treatment of Atoms and Molecules, Hartree- Fock Theory: 12 Review of the principles of quantum mechanics Bom-Oppenheimerapproximation Sister-Condin rules. Hartree-Fockacuation Koopmans and Brifouintheories, Roothan equation, Gaussian basis sets.

ii. Configuration Interaction and MC-SCF: 12

Introduction to Ci, full and truncated Cl theories, size consistency. Introductory treatment of coupled cluster and MC-SCF methods.

iii. Semi-Empirical Theories: 12

A review of the Huckel, EHT and PPP treatments,ZDO approximation, detailed treatment of CNDO and INDO theories. A discussion of electronic energies and properties. An introduction to MCPAC and AMI with hands on experience on personal computers

iv. Density Functional Theory: 12

Derivation of Hohenberg-Kohn thaorom Kohn-Sham formulation, N. and V representablises; review of the performance of the existing incal (eg.SaterXa and other methods) and non-local functionals, treatment of chemical concepts with the density functional theory.

v. Computer Experiments: 12

Computer experiments using quantum chemistrysoftware packages much as GAUSSIAN GAMESS/MOPAC and modeling software egMM2/AMBER/CHARM.

Books Recommended

i. **N.S. Oetune and A. Sabo,** *"MadenQuartien Chemistry",*McGow Hill.

ii. **R.G. Parr and W, Yang,***"Density Functional Theory of Atoms and Molecules",* Oxford.

iii. **J.B. Foresman and E.Frish,***"Exploring g Chemistry with Electron Structure Mithos*",Goussian

Inc.

iv. **Pople and D.L.Beveridge ,***"Semi-empirical MO Theory"*.

v. **R. Mc Weeny and BT. Sutcliffe,** *"Methods of Molecular Quantum Mechanics*", Academic

Press.

Practical

IX Semester

CHY- 905: Practical (Organic, Inorganic & Physical Chemistry)

(18 hrs/week)

CHY-702: Inorganic Chemistry

Paper Type: Practical Total Hours: 270Hrs

Paper type: core Total Credits: 4

Objective:

Impart training in operating different instruments used in the analysis of various chemical constituents.

Course Outcomes:

After successful completion of this course, students will be able:

CO1: Design chromatographic and titrimetric methods for identification of species.

CO2: Analyze different constituents through instrumental methods of analysis.

CO3: Preparation of inorganic compounds and their studies by I.R., Electronic spectra, and Mossbauer spectroscopy

CO4: To study surface tension-concentration relationship for solutions (Gibbsequation).

CO5: Isolation of caffeine from tea leaves.

Unit- 1: Inorganic Preparations:

Preparation of selected inorganic compounds and their studies by I.R., Electronic spectra, Mossbauer, E.S.A. and magnetic susceptibility measurements. Handling of air and moisture sensitive compounds-

i.$VO(acac)_2$

ii.$TiO(C_9H_8NO)_2.2H_20$

iii. cis-$K[Cr(C_20_4)_2(H_20)_2]$

iv.$Na[Cr(NH_3)_2(SCN)_4]$

v.$Mn(acac)_3$

vi.$K_3[Fe(C_20_4)_3]$

vii.PrussianBlue,Turnbull'sBlue.

viii.$Co(NH_3)_6][Co(N0_2)_6]$.

ix. cis-$[Co(trien)(N0_2)_2]Cl..H_20$

x. $Hg[Co(SCN)_4]$ xi. $[Co(Py)_2Cl_2]$

xii.$[Ni(NH_3)_6]Cl_2$ xiii.$Ni(DMG)_2$

xiv.$[Cu(NH_3)_4]S0_4.H_20$

Unit- 2: Organic Chemistry

A. Organic Qualitative Analysis:

Separation, purification and identification of the components of a mixture of three organic compounds (three solids or two liquids and one solid, two solids and one liquid), using tic for checking the purity of the separated compounds, chemical analysis, IR, PMR and mass spectral data.

B. Extraction of Organic Compounds from Natural Sources

i. Isolation of caffeine from tea leaves.

ii. Isolation of casein from milk (the students are required to try some typical color reactions of proteins).

iii. Isolation of lactose from milk (purity of sugar should be checked by TLC and PC and Rf value reported).

iv. Isolation of nicotine dipicrate from tobacco. Isolation of cinchonine from cinchona bark

v. Isolation of piperine from black pepper.

vi. Isolation of lycopene from tomatoes.

vii. Isolation of ß-carotene from carrots.

viii. Isolation of oleic acid from olive oil (involving the preparation of complex with urea and separation of linoleic acid).

ix. Isolation of eugenol from cloves.

x. Isolation of (+) limonine from citrus rinds

Paper Chromatography:

Separation and identification of the sugars present in the given mixture of glucose, fructose and sucrose by paper chromatography and determination of Rf values.

Unit- 3: Physical Chemistry:

A. Error Analysis and Statistical Data Analysis:

Errors, types of errors, minimization of errors, error distribution curves, precision, accuracy and combination; statistical treatment for error analysis, student 't' test, null hypothesis, rejection criteria, F & Q test; linear regression analysis,curve fitting.

Apparatus:burette,pipette, stand and flask.

B. Adsorption:

i. To study surface tension-concentration relationship for solutions (Gibbsequation).

ii. Study the adsorption of acidic acid on charcoal and draw the freundlich isotherm

Books Recommended

i. **J. Derek Woollins,** *"Inorganic Experiments"*, VCH.

ii. **Z. Szafran, R. M. Pike and M. M. Singh,** *"Microscale Inorganic Chemistry"*, Wiley.

iii. **G. Marr and B. W. Rockett,** *"Practical Inorganic Chemistry"*, Van Nostrand.

iv. **J. Bassett. R.C. Denney, G.H. Jeffery and J. Mendham,** *"Vogel's Textbook of Quantitative Analysis"*, revised. ELBS.

v. **W.L. Jolly,** *"Synthesis and Characterization of Inorganic Compounds",* Prentice Hall.

vi. **R. L. Shriner and D. Y. Curtin,** *"The Systematic Identification of Organic Compounds"*.

vii. **D. Pasto, C. Johnson and M. Miller,** *"Experiments and Techniques in Organic Chemistry",* PrenticeHall.

viii. **K.L. Williams on, D.C. Heath,** *"Macro scale and Micro scale Organic Experiments"*.

ix. **H. Middleton, Adward Arnold,** *"Systematic Qualitative Organic Analysis"*.

x. **H. Clark, Adward Arnold,** *"Handbook of Organic Analysis, Qualitative and Quantitative".*

xi. **A.R. Tatchell,** *"Vogel's Textbook of Practical Organic Chemistry",* John Wiley.

xii. **A.M. James and F, E. Prichard,** *"Practical Physical Chemistry"*, Longman.

xiii. **B.P. Levitt,** *"Findley's Practical Physical Chemistry",* Longman.

xiv. **R.C. Das and B. Behera,** *"Experimental Physical Chemistry",* Tata Mc Graw Hill.

xv. **J J. Fisch and R B. King,** *"Organametallic Synthesis*", Academic.

xvi. **D. P. Shoemaker, C. W. Garland and J. W. Niber**, *"Experimental Physical Chemistry",* McGraw Hill Interscience.

xvii. **J. C, Ghosh,** *"Experiments in Physical Chemistry"*, Bharati Bhavan.

Marks Distriution		**Max. Marks**
1.	Inorganic Experiment	20
2.	Organic Experiment	20
3.	Physical Experiment	20
4.	Record	8
5.	Viva- voce	7
Total:		75

SEMESTER – X

Paper -1

CHY - 1001: Photochemistry/ Solid State

Paper Type: Theory Total Hours: 60

Paper type: Core *Total Credits: 4*

Objective:

The objective of the core paper is to study the photochemical reaction and their stereochemistry. Along with this student will get the knowledge in about crystal structure, stoichiometry and solid state reaction.

Course Outcomes:

After successful completion of this course, students will be able:

CO1: Photochemistry:

(A) Photochemical Reactions.
(B) Determination of reaction mechanism.
(C) Photochemistry of Alkenes.
(D) Photochemistry of Carbonyl Compounds.
(E) Photochemistry of aromatic compounds.
(F) Miscelleneous photochemical reactions.

CO2: Solid State:

(A) Solid State reactions.
(B) Crystal defects and non-stoichiometry

(C) Electronic properties and band theory

1.Photochemistry:

A. Photochemical Reactions: 4

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

B. Determination of reaction mechanism: 4

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-photo dissociation, gas-phase photolysis**.**

C. Photochemistry of alkenes: 6

Intramolecular reactions of the olefinic bond- geometrical isomerization, cyclic reactions, rearrangement of 1,4- and 1,5- dienes.

D. Photochemistry of carbonyl compounds: 8

Intramolecular reactions of thecarbonyl compounds- saturated, cyclic and acyclic, β-γ Unsaturated and α-βunsaturated compounds, cyclohexadienones, intermolecular cycloaddition reactions-dimerisation and oxectane formation.

E. Photochemistry of aromatic compounds: 4

Isomerization, addition andsubstitutions.

F. Miscellaneous photochemical reactions: 4

Photo-fries reactions of anilides, photo-fries rearrangement, Barton reaction, singlet molecular oxygen reactions,photochemical formation of smog, photo degradation of polymers, photochemistry of vision.

2.Solid State Chemistry:

Solid State reactions: 4

General principles, experimental procedures, co- precipitation as a precursor to solid-state reactions, kinetics of solid-state reactions.

A. Crystal Defects and Non-Stoichiometry: **6**Perfect and imperfect crystals,intrinsic andextrinsic defects-point defects, line and plane defects, Vacancies- Schotty defects and Frenkel defects, thermodynamics of Schotky and Frenkel defect formation, color centers, non-Stoichiometry and defects.

B. Electronic properties and band theory: 15

Metals, insulators and semiconductors, electronic structure of solid-band theory, band structure of metals, insulators and semiconductor, intrinsic and extrinsic semiconductors, doping semiconductor, p-n-junction, super conductors, optical properties-optical properties - optical reflectance, photoconduction- photoelectric effects, magnetic propertiesclassification of materials: quantum theory of paramagnetic-cooperative phenomena-magnetic domains, hysteresis.

C. Organic solids: 5

Electrically conducting solids, organic charge transfers complex, organic metals, new superconductors.

Books Recommended

i. **K. K. Rohtagi-Mukherji,** *"Fundamentals of Photochemistry"*, Wiley Eastern.

ii. **A. Gilbert and J. Baggott,** *"Essentials of Molecular Photochemistry*", Blackwell Scientific Publication.
iii. **N. J. Turro, W. A. Benjamin,** *"Molecular Photochemistry"*.
iv. **C.H. Depuy and O.L. Chapman,**"*Molecular Reactions and Photochemistry"*, 2nd Edition (1988), Prentice-Hall of India (P) Ltd.,New Delhi.
v. **F.A. Carey and R.J. Sundberg,**"*Photochemistry* in *Advanced Organic Chemistry"*, Chapter 13, Part A, 3rd Edition (1990), Plenum Press, New York.
vi. **A. Cox and T. Camp,** *"Introductory Photochemistry",* McGraw-Hill
vii. **L.V. Azaroff,**"*Singapore Introduction to Solids"*, (1977), Tata McGraw-Hill, New Delhi.
viii. **A.R. West,** "Solid State Chemistry and its Applications" (1984),John Wiley and Sons.
ix. **L. Smart and E Moore,** *"Solid State Chemistry"* (1992), Chapman & Hall, Madras.
x. **H. V. Keer,** *"Principles of Solid State"*(1993), Wiley Eastern.
xi. **J. Turro,**"*Modern Molecular Photochemistry"*, University Science Books, Sausalito (1991).
xii. **R. P. Kundall and A. Gilbert,** *"Photochemistry"*, Thomson Nelson.
xiii. **D.K. Chakrabarty,** *"Solid State Chemistry"*, New Age International.
xiv. **J. Coxon and B. Halton,** *"Organic Photochemistry"*, Cambridge University Press.
xv. **N.B. Hannay,** *"Solid State Chemistry"*,

Additional References

1 **M.B. Smith and J. March,** "*March's Advanced Organic Chemistry-Reactions, Mechanisms and Structure"*, 5th Edition (2001), John Wiley & Sons, New York.
2 **D. Nasipuri**, "*Stereochemistry of Organic Compounds"*, 2nd Edition (1994), Wiley Eastern Ltd., New Delhi.
3 **J. Aube and R. E. Gawley,**"*Principles of Asymmetric Synthesis"*.
4 **Paul de Mayo,**"*Molecular Rearrangements"*, Vol.I& II, Interscience Publishers, New York (1963).
5 **John D. Coyle,**"*Introduction to Organic Photochemistry"*, John Wiley and Sons, New York (1986).
6 **E.L. Eliel, S.H. Wilen and L.N. Mander**, "*Stereochemistry of Organic Compounds"*, Wiley Interscience, New York (2004).

Paper -2

CHY1002 Environmental Chemistry

Paper Type: Theory — Total Hours: 60

Paper type: Core — *Total Credits: 4*

Objective:

The objective of this paper is to study the impact of industry and infrastructure on the environment. Environmental chemistry offers the skils and expertise to enter field like energy and consultancy, public health, environmental risk assessment and pollution control.

Course Outcomes:

After successful completion of this course, students will be able:

CO1: Study of Environment.

CO2: Study of Hydrosphere.

CO3: Study of Soils

CO4: Study of Atmosphere

CO5: Study of Industrial Pollution

CO6: Study of Environmental Toxicology

1. Environment: 12

Introduction composition of atmosphere, vertical temperature, heat budget of the earth atmospheric system,vertical stability atmosphere, and biogeochemical cycles of C, N, P, S and O, Bio distribution of elements.

2. Hydrosphere: 10

Chemical composition of water bodies – lakes, streams, rivers andwetlands etc Hydrological cycle. Aquatic pollution-inorganic, organic, pesticides,agricultural, industrial and sewage, detergents, oil spills and oil pollutants, water quality parameters-dissolved oxygen, biochemicaloxygen demand, solids, metals, content of chloride, sulphate, phosphate, nitrate and micro-organisms, water qualitystandards, Analytical methods for measuring BOD, DO, COD, F, OILS, METALS (As, Cd, Cr, Hg, Pb, Se), Residual chloride and chlorine demand, purification andtreatment of water.

3. Soils: 6

Composition, micro and macronutrients, pollution-fertilizers, pesticides, plastics andmetals, waste treatment.

4. Atmosphere: 8

Chemical Composition of Atmosphere-particles, ions and radical and photochemical reactions in atmosphere, smog formation, oxides of N, C, S, O and their effect, pollution by chemicals, petroleum, minerals, chlorofluorohydrocarbons, greenhouse effect, acid rain, air pollution controls and their chemistry, analyticalmethods for measuring air pollutants, continuous monitoring instruments.

5. Industrial pollution: 12

Cement, sugar, distillery, drug, paper and pulp, thermal power plants, nuclear power plants, metallurgy, polymers, drugs etc, radionuclide analysis, disposal of wastes and their management

.

6. Environmental Toxicology: **12**

Chemical solutions to environmental problems, bio- degradability, principles of decomposition, better industrial processes.

Books Recommended

1. **Stanley Manahan,**"Environmental Chemistry", 10th Edition, CRC Press, Tayler& Frances Group.
2. **Anil Kumar De and Arnab Kuar De,** *"Environmental Chemistry"*, 4th Edition (2000), New AgePublication International Private Ltd.,New Delhi.
3. **Balram Pani,** *"Text Book of Environmental Chemistry"*, 2nd Edition, Wiley Publication.
4. **G.W. Vanloon, S.J. Duffer,** *"Environmental Chemistry" - A Global Perspective*, Oxford University Press (2000).
5. **F.W. Fifield and W.P.J. Hairens,**"*Environmental Analytical Chemistry"*, 2nd Edition (2000), Black Well Science Ltd.
6. **Colin Baird,** *"Environmental Chemistry"*, W.H. Freeman and Company, New York (1995).
7. **Peter O. Warner,** "*Analysis of Air Pollutants",* 1st Edition (1996), John Wiley, New York.
6. **S.M. Khopkar,**"*Environmental Pollution Analysis",* 1st Edition (1993), Wiley Eastern Ltd., New Delhi.
7. **SamirkK. Banerji,**"*Environmental Chemistry",* 2nd Edition,Learning Meripustak,Prentice-Hall of India, New Delhi.
8. **S. E. Manahan,***"Environmental Chemistry"*, Lewis Publishers.
9. **F.J. Welcher,***"Standard Method of Chemical Analysis*", Vol. III, Van Nostrand Reinhold Co.
10. **Ed. J. Rose,***"Environmental Toxicology",* Gordon and Breach Science Publication.
11. *"Environmental Chemistry"*, IGNOW study guide book, MEV-013, Gyaniversity.
12. **B.K. Sharma,***"Environmental Chemistry*", Krishna PrakashanPublication Media Pvt Ltd.
13. Fundamental Concepts of Environmental Chemistry third Edition, Norosa Publication House, G.S. Sodhi.
14. **Dr. S. S. Dara and Dr. D.D. Mishra,***"Text Book of Environmental Chemistry and Pollution Control,* S. Chand Publication.
15. **Ed. S. Landsberger and M. Creatchman,***"Elemental Analysis of Airborne Particles*", Gordon and Breach Science Publication.

Paper -3

CHY-10031: Medicinal Chemistry

Paper Type: Theory Total Hours: 60

Paper Type: Elective Paper-I Total Credits: 4

Objective:

Medicinal chemistry provides chemistry students with a thorough understanding of drug mechanisms of action, structure-activity relationships (SAR), acid-base and physicochemical properties, and absorption, distribution, metabolism, excretion, and toxicity (ADMET) profiles.

Course Outcomes:

After successful completion of this course, students will be able:

CO1:Drug design
CO2: Pharmacokinetics
CO3: Pharmacodynamics
CO4: Antineoplastic agents
CO5: Cardiovascular drugs
CO6 : Local antiinfective drugs
CO7: Psycoactive drugs-the chemotherapy of mind

1. Drug Design: 10

Development of new drugs, procedures followed in drug design, concepts of load compound and lead modification, concepts of prodrugs and soft drugs, structure-activity relationship (SAR). factors affecting bloactivity, resonance, Inductive effect, isosterism, bioleosteriem,spatialconsiderations. Theories of drug activity: occupancy theory, rate theory, induced fit theory. Quantitative structure activity relationship. History and development of QSAR. Concepts of drug receptors. Elementary treatment of drug receptor interactions. Physico-chemical parameters: lipophilicity, partition coefficient, electronic ionization constants, steric, Shelton and surface activity parameters and redox potentials. Free-Wilson analysis, Hansch analysis, relationships between Free-Wilson and Hanschanalysis. LD_{50}, ED_{50} (Mathematical derivations of equations excluded).

2. Pharmacokinetics: 5

Introduction to drug absorption, disposition, elimination using pharmacokinetics, important pharmacokinetic parameters in defining drug disposition and in therapeutics. Mention of uses of pharmacokinetics in drug development process.

3. Pharmacodynamics: 5

Introduction, elementary treatment of enzyme stimulation, enzyme inhibition, sulphonamides, membrane active drugs, drug metabolism, xenobiotics, biotransformation, significance of drug metabolism in medicinal chemistry.

4. Antineoplastic Agents: 10

Introduction, cancer chemotherapy, special problems, role of alkylating agents and antimetabolites in treatment of cancer. Mention of carcinolytic antibiotics and mitotic inhibitors. Synthesis of mechlorethamine, cyclophosphamido, melphalan, uracil, mustards, and 6 mercaptopurine. Recent development in cancer chemotherapy. Hormone and natural products.

5. Cardiovascular Drugs: 5

Introduction, cardiovascular diseases, drug inhibitors of peripheral sympathetic function, central intervention of cardiovascular output. Direct acting arteriolar dilators Synthesis of amyl nitrate, sorbitrate, diltiazem, quinidine, verapamil, methyldopa, atenolol oxyprenolol.

6. Local Antiinfective Drugs: 8

Introduction and general mode of action. Synthesis of sulphonamides, furazolidone, nalidixic acid, ciprofloxacin, norfloxacin, dapsone, amino salicylic acid, isoniazid, ethionamide, ethambutal, fluconazole, econozole, griseofulvin, chloroquin and primaquin.

7. Psychoactive Drugs- The Chemotherapy of Mind: 10

Introduction, neurotransmitters, CNS depressants, general anaesthetics, mode of action of hypnotics, sedatives, anti-anxiety drugs, benzodiazipines, buspirone, neurochemistry of mental diseases. Antipsychotic drugs - the neuroleptics, antidepressants, butyrophenones, serendipity and drug development, stereochemical aspects of psychotropic drugs. Synthesis of diazepam, oxazepam, chlorazepam, alprazolam, phenytoin, ethosuximde, trimethadione, barbiturates, thiopental sodium, glutethimide

8. Antibiotics: 7

Cell wall biosynthesis, inhibitors, B-lactam rings, antibiotics inhibiting protein synthesis Synthesis of penicillin G, penicillin V. ampicillin, amoxycillin, chloramphenicol, cephalosporin, tetracyclin and streptomycin.

Books Recommended

i. **A.Gringuage,** *"Introduction to Medicinal Chemistry",* Wiey-VCH.

ii. **Ed Robert F.Dorge,** *"Wilson and Gisvold's Text Book of Organic Medicinal and Pharmaceutical Chemistry".*

iii. **S. S. Pandeya and J. R. Dimmock,** *"An Introduction to Drug Design"*, New Age International.

iv. **Ed. M. E. Wolff,** *"Burger's Medicinal Chemistry and Drug Discovery",* Vol-1 (Chapter-9 and Ch-

14), John Wiley.

v. **Goodman and Giman's,** *"Pharmacological Basis of Therapeutics"*, McGraw-Hill.

vi. **R. B. Silverman,** *"The Organic Chemistry of Drug Design and Drug Action"*, Academic Press.

vii. **D. Lednicer,** *"Strategies for Organic Drug Synthesis and Design*", John Wiley.

Additional References

1. **A. Burger,** *"Medicinal Chemistry"*, Vol. I-III, (1995) Wiley Interscience Publications, New York.
2. **W. O. Foye,**"*Principles of Medicinal Chemistry"*, 3rdEdition (1989), Lea &Febiger/ Varghese Publishing House, Bombay.
3. **D. Lednicer and L. A. Mitscher,**"*The Organic Chemistry of Drug Synthesis"*, (1977) Vol. I-III, Wiley Interscience.
4. **A. Kar,** *"Medicinal Chemistry"*, (1993) Wiley Eastern Ltd., New Delhi.
5. **N. K. Terrett,**"*Combinatorial Chemistry",* (1998) Oxford Univ. Press, Oxford.
6. **Daniel Lednicer**,"*Stretegies for Organic Drug Synthesis and Design"*(2009),John Wiley & Sons, New York.

Paper -3

CHY-10032: Chemistry of Materials

Paper Type: Theory Total Hours: 60

Paper Type: Elective Paper-I Total Credits: 4

Objective:

Material chemistry deals with the multiphase material and their applications.The most important application focuses polymer composite with the nanomaterials.

Course Outcomes:

After successful completion of this course, students will be able:

CO1:Development of multiphase material and properties of ferrous and non-ferrous alloys and their applications.

CO2: Characteristic of composite with nanomaterials.

CO3: Mesmorphic behaviour, thermotropic liquid crystals, positional order, bond orientational order, nematic and smectic mesophases of liquid crystals.

CO4: Molecular shape, structure and configuration, crystallinity, stress-strain behaviour, thermal behaviour, polymer types and their applications, conducting and ferro-electric polymers.

CO5: Conducting organics, organic superconductors, magnetism in organic materials. Fullerenes-doped, fullerenes as superconductors

1. Multiphase Materials: 5

Ferrous alloys; Fe-C phase transformations in ferrous alloys; stainless stools, non- ferrous alloys, properties of ferrous and non-ferrous alloys and their applications.

2. Glasses, Ceramics, Composites and Nanomaterials: 7

Glassy state, glass formers and glass modifiers, applications. Ceramic structures, mechanical properties, clay products. Refractories, characterizations, properties and applications. Microscopic composites; dispersion-strengthened and particle-reinforced, fibre-reinforced composites, macroscopic composites. Nanocrystalline phase, preparation procedures, special properties, applications.

3. Thin Films and Langmuir-Blodgett Films: 5

Preparation techniques; evaporation/sputtering, chemical processes, MOCVD, sol-gel etc. Langmuir-Blodgett (LB) film, growth techniques, photolithography, properties and applications of thin and LB films.

4. Liquid Crystals: 10

Mesmorphicbehaviour, thermotropic liquid crystals, positional order, bond orientational order, nematic and smectic mesophases: smectic nomatic transition and clearing temperature- homeotropic, planar and schlieren textures, twisted nematics, chiral nematics, molecular arrangement in smectic A and smectic C phases, optical properties of liquid crystals.Dielectric susceptibility and dielectric constants. Lyotropic phases and their description of ordering in liquid crystals.

5. Polymeric Materials: 5

Molecular shape, structure and configuration, crystallinity, stress-strain behaviour, thermal behaviour, polymer types and their applications, conducting and ferro-electric polymers.

6. Ionic Conductors: 8

Types of ionic conductors, mechanism of ionic conduction, interstitial jumps (Frenkel). vacancy mechanism, diffusion superionic conductors: phase transitions and mechanism of conduction in superionic conductors, examples and applications of ionic conductors.

7. High Tc Materials: 8

Defect perovskites, high Tc superconductivity in cuprates, preparation and characterization of 1-2-3 and 2-1-4 materials, normal state properties; anisotropy; temperature dependence of electrical resistance; optical phonon modes, superconducting state; heat capacity. coherence length, elastic constants, position lifetimes, microwave absorption-pairing and mutti gap structures in high Tc materials, applications of high Tc materials.

8. Materials for Solid State Devices: 3

Rectifiers, transistors, capacitors -IV-V compounds, low-dimensional quantum structures: optical properties.

9. Organic Solids, Fullerenes, Molecular Devices: 9

Conducting organics, organic superconductors, magnetism in organic materials. Fullerenes-doped, fullerenes as superconductors. Molecular rectifiers and transistors, artificial photosynthetic devices, optical storage memory and switches-sensors. Nonlinear optical materials: nonlinear optical effects. second and third order molecular hyperpolarisability and second order electric susceptibility- materials for second and third harmonic generation.

Books Recommended

i. **N.W. Ashcroft and N.D. Marmin,** *"Solid State Physics",* Saunders College.
ii. **W.D.Calister,** *"Material Science and Engineering, An Introduction",* Wiley.
iii. **H.V. Keer,** *"A Principles of the Solid State*", Wiley Eastem.
iv. **J.C. Anderson, K.D. Leaver, J.M. Alexander and R.D. Rawlings,** *"Materials Science*", ELBS.
v. **Ed. G.W. Gray,** "*Thermotropic Liquid Crystals*", John Wiley.
vi. **Keteer and Hatz,** *"Handbook of Liquid Crystals"*, ChemieVerleg.

Paper-3

CHN-10033: Organic Synthesis II

Paper Type: Theory Total Hours: 60

Paper Type: Elective Paper-I Total Credits: 4

Objective:

Organic synthesis involves strategies for making compounds from readily available starting materials by one or more steps. The heart of organic synthesis is designing synthetic routes to a molecule.Selectivity is an important consideration when determining a synthetic route to a target molecule. Chemists need to consider both stereoselectivity and chemoselectivity in organic synthesis.Synthetic reactions can be categorized based on whether they involve functional group interconversion or carbon-carbon bond formation.

Course Outcomes:

After successful completion of this course, students will be able:

CO1 : Discuss the terminology, criteria for selecting target, synthesis involving chemo and regio selectivity, reversal of polarity and cyclisation involved in retro synthesis analysis.
CO2 : Explain order of events, one bond and two bond C-C and C-X disconnection and control in carbonyl condensation with examples.
CO3 : Discuss the types of asymmetric synthesis controlled by chiral auxiliary, chiral catalyst, chiral substrate and chiral reagent with examples.

CO4 : Define strategic bond and discuss guidelines for disconnection with greatest simplification using symmetry and corresponding to known reliable reactions, Retro synthesis of Retronecene, Longifoline.

Disconnection Approach: **1.** An introduction to synthons and synthetic equivalents, disconnectionapproach, functional group inter-conversions, the importance of the order of events in organic synthesis, one group C-X and two group C-X disconnections, chemoselectivity, reversal of polarity, cyclisation reactions, amine synthesis.

2. **Protecting Groups:** **7**

Principle of protection of alcohol, amine, carbonyl and carboxyl groups.

3. **One Group C-C Disconnections** **9**

Alcohols and carbonyl compounds, regioselectiviity. Alkene synthesis, use ofacetylenes and aliphatic nitro compounds in organic synthesis.

4. **Two Group C –C Disconnections** **12**

Diels-Alder reaction, 1,3-difunctionalised compounds, unsaturated carbonylcompounds, control in carbonyl condensations, 1,5-difunctionalised compounds, Michael addition and Robinson annulations.

5. **Ring Synthesis:** **8**

Saturated heterocycles, synthesis of 3-, 4-, 5- and 6-membered rings, aromatic heterocycles in organic synthesis.

6. **Synthesis of Some Complex Molecules :** **12**

Application of the above in the synthesis of following compounds: Camphor, Longifoline, Cortisone, Reserpine, Vitamin D, Juvabione, Aphidicolin and Fredericamycin A.

Books Recommended

i. **S. Warren,** *"Designing Organic Synthesis*", Wiley.

ii. **J.Fuhrhop and G. Penzillin,** *"Organic Synthesis- Concept, Methods and Starting Materials"*, VerlageVCH.

iii. **W. Carruthers,** *"Some Modern Methods of Organic Synthesis"*, Cambridge Univ. Press.

iv. **H.O.House,** *"Modern Synthetic Reactions"*, W. A. Benjamin,

v. **J. March,** *"Advanced Organic Chemistry: Reactions, Mechanisms and Structure*",Wiley.

vi. **A. Norman and J. M. Coxon,** *"Principles of Organic Synthesis"*, Blackie Academic & Professional.

vii. **F. A. Carey and A. J. Sundberg,** *"Advanced Organic Chemistry -Part B*", Plenum Press.

Paper-3

CHY-10034 Physical Organic Chemistry

Paper Type: Theory Total Hours: 60

Paper Type: Elective Paper-I Total Credits: 4

Objectives

The course deals with fundamental principles and methods used in physical and mechanistically organic chemistry

Course Outcomes:

After successful completion of this course, students will be able:

CO1: apply qualitative electronic structure theory to predict the geometric structure, reactivity and other properties of organic molecules (including organometallic compounds and conjugated polymers), and to apply qualitative theoretical models to describe pericyclic reactions.
CO2: predict conformational preference of organic molecules and the stereochemical preference in reactions
CO3: critically evaluate and apply different techniques for the determination of mechanisms of organic reactions
CO4: describe different types of reactive intermediates and describe their importance in different reactions
CO5: apply fundamental concepts of chemical and biochemical catalysis
CO6: describe various forms of non-covalent interactions in organic, bioorganic and supramolecular systems, and predict the influence of solvent on reactivity
CO7: describe important processes of organic molecules in electronically excited.

1.Concepts In Molecular Orbital (MO) and Valence Bond (VB) Theory: 10

Introduction to Huckel molecular orbital (MO) method as a means to explain modern theoretical methods.Advanced techniques in PMO and FMO theory.Molecular mechanics, semi empirical methods and ab inito and density functional methods. Scope and limitations of several computational programmes. Quantitative MO theory - Huckel molecular orbital (HMO) method as applied to ethene, allyl and butadiene. Qualitative MO theory lonisation potential. Electron affinities. MO energy levels. Orbital symmetry. Orbital Interaction diagrams. MO of simple organic systems such as ethene, allyl, butadiene, methane and methyl group. Conjugation and hyperconjugation. Aromaticity.Valence bond (VB) configuration mixing diagrams. Relationship between VB configuration mixing and resonance theory. Reaction profiles. Potential energy diagrams. Curve crossingmodel-nature of activation barrier in chemical reactions

2. Principles of Reactivity:5

Mechanistic significance of entropy, enthalpy and Gibb's free energy. Arrhenius equation. Transition state theory. Uses of activation parameters, Hammond's postulate, Bell-Evans Polanyi principle. Potential energy surface model. Marcus theory of electron transfer. Reactivity and selectivity principles.

3. Kinetic Isotope Effect: 4

Theory of isotope effects. Primary and secondary kinetic isotope effects. Heavy atom isotope effects. Tunneling effect. Solvent effects.

4. Structural Effects on Reactivity: 6

Linear free energy relationships (LFER). The Hammett equation, substituent constants, theories of substituent effects. Interpretation of a-values, Reaction constant p. Deviations from Hammett equation. Dual-parameter correlations, inductive substituent constant. The Taft model, ar- and de-scales.

5. Solvation and Solvent Effects: 6

Qualitative understanding of solvent-solute effects on reactivity. Thermodynamic measure of solvation. Effects of solvation on reaction rates and equilibria. Various empirical indexes of solvation based on physical properties, solvent-sensitive reaction rates, spectroscopic properties and scales for specific solvation. Use of solvation scales in mechanistic studies. Solvent effects from the curve-crossing model.

6. Acids, Bases, Electrophiles, Nucleophiles and Catalysis: 6

Acid-base dissociation. Electronic and structural effects, acidity and basicity. Acidity functions and their applications. Hard and soft acids and bases. Nucleophilicity scales. Nucleofugacity. The a-effect. Ambivalent nucleophiles. Acid-base catalysis specific and general catalysis. Bronsted catalysis. Nucleophilic and electrophilic catalysis, Catalysis by non-covalent binding-micellar catalysis.

7. Steric and Conformational Properties: 6

Various type of steric strain and their influence on reactivity. Steric acceleration, Molecular measurements of steric elfects upon rates. Steric LFER. Conformational barrier to bond rotation-spectroscopic detection of individual conformers. Acyclic and monocyclic systems.

Rotation around partial double bonds. Winstein-Holness and Curtin-Hammett principle.

8. Nucleophilic and Electrophilic Reactivity: 6

Structural and electronic effects on S1 and S2 reactivity. Solvent effects Kinetic isotope effects. Intramolecular assistance. Electron transfer nature of S2 reaction. Nucleophilicity and S2 reactivity based on curve- crossing model. Relationship between polar and electron transfer reactions. Saw mechanism, Elecrophilic reactivity, general mechanism, Kinetic S2- Ar reaction. Structural effects on rates and selectivity Curve-crossing approach to electrophilic reactivity.

9. Radical and Pericyclic Reactivity: 6

Radical stability, polar influences, solvent and steric effects. A curve crossing approach to radicat addition, factors effecting barrier heights in additions, regioselectivity in radical reactions, Reactivity, specificity and periselectivity in pericyclic reactions.

10. Supramolecular Chemistry: 5

Properties of covalent bonds bond length inter-bond angles, force constant, bond and molecular dipole moments Molecular and bond polarizability, bond dissociation enthalpy. entropy. Intermolecular forces, hydrophobic effects Electrostatic, induction, dispersion and resonance enorgy magnetic interactions. magnitude of interaction energy, forces between macroscopic bodies, medium effects Hydrogen bond Principles of molecular association and organization as exemplified in biological macromolecules ke enzymes nucleic acids, membranes and model systems like micelles and vesicles Molecular receptors and design principles Cryptands, cyclophanes. calixeranes, cyclodextrines. Supramolecular reactivity and catalysis. Molecular channels and transport processes. Molecular devices and nanotechnology.

Books Recommended

i. **U. Burkert and N. L. Allinger,** *"Molecular Mechanics"*, ACS Monograph 177, 1982.

ii. **L. Salem and W. L. Jorgensen,** *"Organic Chemists Book of Orbitals*". Academic Press.

iii. **T. H. Lowry and K. C.Richardson, and Row,** *"Mechanism and Theory in Organic Chemistry".* iv. **W. B. Smith,** *"Introduction to Theoretical Organic Chemistry and Molecular Modeling",* VCH,
Weinheim.

v. **N. S. Isaacs,** *"Physical Organic Chemistry"*, ELBS/Longman.

vi. **J. M, Lehn,** *"Supramolecular Chemistry: Concepts and Perspectives",* VCH.

vii. **H. Maskill,** *"The Physical Basis of Organic Chemistry*", Oxford University Press.

Paper-4

CHY-1004: Elective Papers II

CHY-10041: Polymer Chemistry

Paper Type: Theory Total Hours: 60

Paper Type: Elective Paper-II Total Credits: 4

Objective:

Objective of the course is the complete knowledge of the kinetics, thermodynamics of polymerization, various techniques of determination of molecular mass and applications of polymers in various fields of life will be provided to the students. Various factors affecting the structure and properties of polymers will be discussed in detail which makes students aware of the things to be considered while preparing polymers commercially.

Course Outcomes:

After successful completion of this course, students will be able:

CO1: The basic concepts of monomers, degree of polymerization, and classification of polymers are the backbone of polymer chemistry.

CO2: This will also help to develop skills to interpret and explain various factors affecting structure and property of macromolecules.

CO3: To understand the concept of macromolecules and determination of molecular weight of the polymer and their application.

CO4: The students will be able to pursue their career objectives in higher education, scientific research and teaching.

Unit-1: **Basics: 10**

Importance of polymers. Basic concepts: Monomers, repeat units, degree of polymerization. Linear, branched and network polymers. Classification of polymers Polymerization: condensation, addition, radical chain-ionic and co-ordination and co polymerization. Polymerization conditions and polymer reactions. Polymerization In homogeneous and heterogeneous systems.

Unit-2: Polymer Characterization: 14

Polydispersion-average molecular weight concept. Numbor, weight and viscocity average molecular weights. Polydispersity and molecular weight distribution. The practical significance of molecular weight. Measurement of molecular weights. End-group, viscocity, light scattering, osmotic and ultracentrifugation methods. Analysis and testing of polymers chemical analysis of polymers, spectroscopic methods, X-ray diffraction study. Microscopy. Thermal analysis and physical testing-tensile strength. Fatigue, impact. Tear resistance, Hardness and abrasion resistance.

Unit-3: Structure and Properties: 14

Morphology and order in crystalline polymers-configurations of polymer chains. Crystal structures of polymers. Morphology of crystalline polymers, strain-induced morphology. Crystallization and melting. Polymer structure and physical properties-crystalline melting point Tm-melting points of homogeneous series, effect of chain flexibility and other 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 cross linking. Property requirements and polymer utilization.

Unit-4: Polymer Processing: 10

Plastics, elastomers and fibres. Compounding Processing techniques: Calendering, die casting, rotational casting, film casting, injection moulding, blow moulding, extrusion moulding, thermoforming, foaming. reinforcing and fibre spinning.

Unit-5: Properties of Commerical Polymers: 12

Polyethylene, polyvinyl chloride, polyamides, polyesters, phenolic resins, epoxy resins and silicone polymers. Functional polymers Fire retarding polymers and electrically conducting polymers. Biomedical polymers contact lens, dental polymers, artificial heart, kidney, skin and blood cells.

Books Recommended

1. **F. W. Billmayer,** *"Text Book of Polymer Science"*, 3rd Edition (1984), Jr., Willey-Interscience, New York.
2. **V.R. Gowariker, N.V. Viswanathan and J. Sreedhar,** *"Polymer Science"*, Wiley-Eastem.
3. **P. W. Atkins,** *"Physical Chemistry"*, 8th Edition, Oxford University Press, New York.
4. **G. Odian,** *"Principles of Polymerization*", 3rd Edition (1991), John Wiley, Singapore.

5. **P. Bahadur and N.V. Sastry,** *"Principle of Polymer Sciences",* Narosa Publishing House, New Delhi (2002).

6. **K. Takemoto, Y. Inaki and RM. Ottanbrite,** *"Functional Monomers and Polymers*".

7. **H.R. Alcock and F.W. Lambe,** *"Contemporary Polymer Chemistry*", Prentice Hall.

8. **J.M.G. Cowie,** *"Physics and Chemistry of Polymers"*, Blackie Academic and Professional.

9. **V.R. Gowarikar, N.V. Vishwanathan, J. Shreedhar,** *"Polymer Sciences"*, Wiley Eastern, New Delhi (1986).

Paper-4

CHY - 10042: Computation Chemistry

Paper Type: Theory Total Hours: 60

Paper Type: Elective Paper -II Total Credits: 4

Objective:

Computational chemistry is a branch of chemistry that uses computer simulation to assist in solving chemical problems. It uses methods of theoretical chemistry, incorporated into computer programs, to calculate the structures and properties of molecules, groups of molecules, and solids. It is essential because, apart from relatively recent results concerning the hydrogen molecular ion (dehydrogenate, see references therein for more details), the quantum many-body problem cannot be solved analytically, much less in closed form. While computational results normally complement the information obtained by chemical experiments, it can in some cases predict hitherto unobserved chemical phenomena. It is widely used in the design of new drugs and materials.

Course Outcomes:

After successful completion of this course, students will be able:

CO1: This course will use Fortran 90 exclusively. We will cover the basics of Fortran 90 throughout this semester. You may want to get a good reference of Fortran 90 in hand**.**

CO2: Develop mathematical thinking and problem solving skills associated with research and writing proofs. Get exposure to a wide variety of mathematical concepts used in computer science discipline like probability. Use Graph Theory for solving problems Acquire basic knowledge of sampling and estimation. Understand basic concepts of hypothesis

CO3: This lesson provides a broad overview of the Computer Networking and the Internet. The lesson begins with an overview of the Internet and of networking protocols, introducing several key terms and concepts. Finally, we provide a brief overview of ATM, a networking technology that provides an important contrast with Internet technologies.

CO4: Following this course, students will be able to describe a project life cycle, and can skillfully map each stage in the cycle. Students will describe the time needed to

successfully complete a project, considering factors such as task dependencies and task lengths. Students will be able to develop a project scope while considering factors such as customer requirements and internal/external goals.

Unit-1: Fortran/C Programming and Numerical Methods:
10

Advanced programming features of FORTRAN/C. Basic theory, discussion of algorithms and errors for the following numerical methods. Examples from chemistry should be selected for illustrating the methods. The teacher may select ANY THREE of the following subtopics considering the background of students, available time etc.

A. Solution of Equations:
6

Bisection, regular falsi, Newton-Raphson and related methods for solving polynomial and transcendental equations. Convergence. Errors and ill-conditioning.

B. Linear Simultaneous Equations :
8

Gaussian elimination, Gauss--Seidel method, Gauss-Jordan method. Pivoting strategy. Errors and ill conditioning.

C. Eigenvalues and Matrix Diagonalization :
4

Jacobi and Householder methods, analysis or errors.

D. Interpolation :
4

Newton forward and backward difference, central differenced formulae. Lagrange and Hermite interpolation. Polynomial wiggle problem.

E. Numerical Differentiation:
4

Solution of simple differential equations by Taylor series and Runge-Kutta methods

F. Numerical Integration:
4

Newton-Cotes formulae, Romberg integration, errors in integration formulae. The students should develop computer programs for some of the above numerical methods

Unit-2: Running of Advanced Scientific Packages:
8

The students are expected to get hands on experience of running a few selected advanced level scientific software packages after & boot Introduction to the basic theory and methodology. ab initio quantum chemical packages such as GAUSSIAN GAMES with carefully designed exercises for illustrating various features of the packages Semi- empirical/Dynamics/Simulation packages such as MOPAC, CHARM, AMBER, QUANTA etc. Basic ideas on structure activity relation, drug and catalysis design etc.

Unit-3: Introduction to Networking and Search using Internet : 2

Unit-4: Project: 10

The students will develop utilities such as analysis of spectra, simulation programmes which will supplement laboratory or theory exercises in physical, organic, inorganic chemistry or biochemistry. This list is only indicative and a variety of small projects designed by the teacher based on the interest of the student and capabilities should be worked out.

Books Recommended

i. A.C. Norris, "Computational Chemistry", John Wiley.
ii. R. Rajaraman, "Computer Programming in FORTRAN 77, Prentice Hall.
iii. C. E. Frogberg, "Numerical Analysis", Macmilan.
iv. M.J. Maron, "Numerical Analysis A Practical Approach", John Wiley.
v. H. M. Anta, "Numerical Methods for Scientists and Engineers", Tata McGraw Hill.

Paper -4

CHY-10043: Photo inorganic Chemistry

Paper Type: Theory Total Hours: 60

Paper Type: Elective Paper -II Total Credits: 4

Objective:

Explain the theory and practice of common photochemical and photophysical methods, and be able to execute these experimentally. Also explains theory and application of photocatalysis and explain the environmental impact of atmospheric photochemistry

Course Outcomes:

After successful completion of this course, students will be able:

CO1: Describe the interaction of excited states with their surroundings, and apply theoretical methods for treating excited states.

CO2: Explain and discuss theories for photoinduced electron transfer and excitation energy transfer, and apply these methods in quantitative calculations

CO3: Explain the mechanisms of common photochemical transformations, analyse them theoretically, and describe the significance of conical intersections in photochemical reactions

CO4: Describe photoinduced processes in semiconductors, and explain how these can be used for photophysical energy conversion.

1. Basics of Photochemistry: 12

Absorption, excitation, photochemical laws, quantum yield, electronically excited states life tumes-measurements of the times. Flash photolysis, stopped flow techniques. Energy dissipation by radiative and non-radiative processes, absorption spectra, Franck-Condon principle, photochemical stages-primary and secondary processes

2. **Properties of Excited States 6**

Structura, dipole moment, acid-base strengths, reactivity. Photochemical kinetics calculation of rates of radiative processes. Bimolecular deactivation- quenching

3. Excited States of Metal Complexes 8

Excited states of metal complexes: comparison with organic compounds, electronically excited states of metal complexes, charge-transfer spectra, charge transfer excitations, methods for obtaining charge-transfer spectra **4. Ligand Field Photochemistry 12**Photosubstitution, photooxidation and photoreduction, ability and selectivity. Zero vibrational levels of ground state and excited state, energy content of excred state, zero zero spectroscopic energy, development of the equations for redox potentials of the excited states.

5. Redox Reactions by Excited Metal Complexes 14 Energy transfer under conditions of weak interaction and strong interaction-exciplex formation conditions of the excited states to be useful as redox reactants, excited electron transfer metal complexes as attractive candidates (2.2-bipyridine and 1,10 phenonthroine complexes). Illustration of reducing and oxidising character of Ruthenium (pyridal complex, comparison with Felblpyls: role of spin-orbit coupling-fe time of these complexes. Application of redox processes of electronically excited states for catalytic purposes, transformation of low energy reactants into high energy products, chemical energy into light

6. Metal Complex Sensitizers 8

Metal complex sensitizer, electron relay, metal colloid systems, semiconductor supported metal or oxide systems, water photolysis, nitrogen fixation and carbon dioxide reduction

Books Recommended

i. **A.W. Adamson and P.D. Fischauer,** *"Concepts of Inorganic Photochemistry"*, Wiley

ii. Inorganic Photochemistry, *J. Chem.* Educ, vol 00, no. 10, 1003

iii. **J. Lippan,** Progress Inorganic Chemistry, vol. 30, ed. 5, Wiley.

iv. *Coordination Chem, Revs* 1981, vol 39, 121, 131, 1975 15 321, 1000, 97, 313 5.

v. **V. Batra and V. Caras,** *"Chemistry of Coordination Compounds*", Academic Press 6.

vi. **G. J. Feraud,** "Elements of Inorganic Photochemistry",Wiley.

Paper -4

CHY-10044: Heterocyclic Chemistry

Paper Type: Theory Total Hours: 60

Paper Type: Elective Paper -II Total Credits: 4

Objective:

Their importance in biology, heterocyclic compounds also find wide applications in diverse areas such as in dyes, photosensitizers, coordination compounds, polymeric materials and many more to mention.

Course Outcomes:

After successful completion of this course, students will be able:

CO1: This course aims at providing theoretical understanding of heterocyclic chemistry
CO2: Explain the nomenclature, synthesis and reactivity of heterocyclic compounds
CO3: Discuss the different types of strains, interactions and conformational aspects of nonaromatic heterocycles.
CO4: It includes various methods for ring synthesis and application of those methods for the preparation of specific groups of heterocyclic systems.
CO5: The students will be made familiar with particular properties, reactions, and applications of the most important as well as less common heterocycles
CO6: Will learn the key applications of various heterocyclic compounds in diverse fields.

1. Nomenclature of Heterocycles 4

Replacement and systematic nomenclature (Hantzsch - Widman system) for monocyclic, fused and bridged heterocycles.

2. Aromatic Heterocycles 5

General chemical behavior of aromatic heterocycles, classification (structural type), criteria of aromaticity (bond lengths, ring current and chemical shifts in 1 H NMR-spectra, empirical resonance energy, delocalization energy and Dewar resonance energy,diamagnetic susceptibility exaltations). Heteroaromatic reactivity and tautomerism in aromatic heterocycles

3. Non Aromatic Heterocycles 6

Strain -bond angle and torsional strains and their consequences in small ring heterocycles. Conformation of six-membered heterocycles with reference to molecular geometry, barrier to ring inversion, pyramidal inversion and 1,3-diaxial interaction. Stereo-electronic effects - anomeric and related effects. Attractive interactions - hydrogen bonding and intermolecular nucleophilic- electrophilic interactions.

4. Heterocyclic Synthesis 4

Principles of heterocyclic synthesis involving cyclization reactions and cycloaddition reactions.

5. Small Ring Heterocycles 5

Three-membered and four-membered heterocycles-synthesis and reactions of aziridines, oxiranes, thiiranes, azetidines, oxetanes and thietanes

6. Benzo Fused Five Membered Heterocycles 5

Synthesis and reactions including medicinal applications of benzopyrroles,benzofurans and benzothiophenes

7. Mesoionic Heterocycles 5

General classification, chemistry of some important meso-ionicheterocycles of type-A and B and theirapplications.

8. Six Membered Heterocycles with One Heteroatom 6

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

9. Six-Membered Heterocycles with Two or More Heteroatoms 5

Synthesis and reactions of diazines, triazines, tetrazinesandthiazines

7. **Seven and Large Membered Heterocycles 5**

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

8. **Heterocyclic System Containing P, As, Sb and B 10**

a. **Heterocyclic rings containing phosphorus:** Introduction; nomenclature, synthesis and characteristics of 5- and 6- membered ring systems- phosphorinanes, phosphorines, phospholanes and phospholes.

b. **Heterocyclic rings containing As and Sb:**

Introduction, synthesis and characteristics of S 5 and 6- membered ring systems.

c. **Heterocyclic rings containing B:**

Introduction, Synthesis, reactivity and spectral characteristics of 3-,5- and 6- membered ring systems.

Books Recommended

i. **A. K. Gupta. M. Kumar and V. Gupta,** *"Heterocyclic Chemistry"*, Vol 1-3, Springer Verlag

ii. **T. Eicher and S. Hauptmann,** *"The Chemistry of Heterocycles"*, Thieme

iii. **J. A. Joule, K. Mills and G.F. Smith,** *"Heterocyclic Chemistry",* Chapmanand Hall

iv. **T.L Gilchrist,** *"Heterocyclic Chemistry*",Longman ScietificTechinal

v. **G. A. Newkome and W. W.Paudler,** *"Contemporary Heterocyclic Chemistry*", Wiley-Inter Science.

vi.**A. M. Acheson,** *"An Introduction to the Heterocyclic Compounds",* JohnWiley

vii. **A. A. Katritzky and C. W. Rees.,** *"Comprehensive Heterocyclic Chemistry*", Eds. Pergamon Press.