CMS COLLEGE KOTTAYAM
(AUTONOMOUS)

Affiliated to the Mahatma Gandhi University
Kottayam, Kerala

CURRICULUM FOR POST GRADUATE PROGRAMME

MASTER OF SCIENCE IN CHEMISTRY

UNDER CREDIT AND SEMESTER SYSTEM (CSS)
(With effect from 2019 Admissions)

Approved by the Board of Studies on 30th April 2019

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ACKNOWLEDGEMENTS

The Board of Studies in Chemistry, CMS College Kottayam (Autonomous), has made serious and sincere attempt to make the curriculum of postgraduate programme in Chemistry. There are many personalities whose relentless support and guidance made this syllabus a success. We take this opportunity to express our sincere appreciation to all those who were part of this endeavor for structuring the syllabus of PG programme in Chemistry. Our heartfelt gratitude to Dr. N. J. Rao, former Professor, Indian Institute of Science for the 2-day workshop on curriculum designing and to Dr. T. P. Sasikumar, former Professor ISRO for the 2-day curriculum workshop, and to Dr. C. James, Scott Christian College for the workshop on question bankdesign.

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Smt.Ajitha Chandy
Chairman
Board of Studies

Kottayam
30.04.2019

PREFACE

The objective of the M.Sc. Chemistry programme is to provide the graduates an in-depth knowledge of the scientific basis and the methodology of chemical research. On completing the programme, the students will be able to analyse and solve problems within the broad/specialized field of chemistry. A master's degree in Chemistry equips the graduates with the necessary skills for embarking a research career or for taking up independent leadership and management of complex work and development situations within the field. The M.Sc. Programme in Chemistry combines core and elective theory courses as well as practical courses and an independent research guided by an experienced researcher from the department or a national institute. Adhering onto these objectives, M.Sc. Curriculum revision was carried out with utmost vigilance and care. The curriculum revision committee believes that we have taken care of every academic aspect to arrive at comprehensive syllabus for all the courses. While revising the M.Sc. syllabus, the committee has taken into account the emerging trends in various fields of theoretical and experimental chemistry. The thrust was given to inculcate the spirit of hard work and research aptitude in students to pursue higher education in the nationally/internationally reputed institutions and laboratories. Brain-storming discussions in this matter were carried out among the faculty members of Chemistry department of CMS College and experts from various other Colleges, Universities and Institutions. The board of studies believes that we have taken care of every aspect to arrive at comprehensive syllabus for all the courses that cater to the advance of the students' knowledge, career and future.

REGULATIONS FOR POST GRADUATE PROGRAMMES UNDER CREDIT SEMESTER SYSTEM 2019

Preamble

CMS College Kottayam (Autonomous) was conferred with the Autonomous status as per UGC No.F.22-1/2016(AC) Dtd. 9th March 2016 and Mahatma Gandhi U.O.No.2732/VII/2016/Acad. Dtd.12th May 2016.

REGULATIONS

CMS College Kottayam (Autonomous) follows Credit Semester System (CSS) for the Post Graduate programmes from the Academic year 2019-20. The Post Graduate programmes of the college are being redesigned and revised in tune with the modifications effected at the UGC Curriculum Framework. This will be reflected in the scheme, course content and mode of examination and Evaluation system. The scheme and syllabus of all the programmes are being revised accordingly. The revisions were effected based on the recommendations made at the Curriculum Revision workshops conducted for the purpose besides several sittings of the Curriculum Revision Committee.

1. TITLE

1.1. These regulations shall be called **"CMS COLLEGE KOTTAYAM (AUTONOMOUS) REGULATIONS FOR POST GRADUATE PROGRAMMES UNDER CREDIT AND SEMESTER SYSTEM 2019"**

2. SCOPE

2.1 Applicable to all regular Postgraduate Programmes conducted by the CMS College Kottayam (Autonomous) with effect from 2019 admissions.

2.2 Medium of instruction is English unless otherwise stated therein.

3. DEFINITIONS

3.1. **Academic Week** is a unit of five working days in which the distribution of work is organized from day one to day five, with five contact hours of one hour duration on each day.

3.2. **Semester** means a term consisting of **90** working days, within **18** five-day academic weeks for teaching, learning and evaluation.

3.3. **Programme** means a two year programme of study and examinations, spread over four semesters, with a set of courses, the successful completion of which would lead to the award of a degree.

3.4. **Course** comprises a set of classes or a plan of study on a particular subject which will be taught and evaluated within a semester of a study programme.

3.5. Core course means a course which should compulsorily be studied by a student as requirement in the subject of specialization within a degree programme.

3.6. Elective Course means an elective course chosen from the discipline/ subject, in an advanced area.

3.7. Credit is the numerical value assigned to a course according to the duration of the classes or volume of the syllabus of the course**.**

3.8. Department means any teaching department in the college.

3.9. Dean of Academic Affairs is a teacher nominated by the Academic Council to coordinate the academic affairs of the college relating to academic planning, curriculum implementation and review.

3.10. Dean of Student Affairs is a teacher nominated by the Academic Council to coordinate the admissions, grievances and other student related services.

3.11. Department Council means the body of all teachers of a department in the college.

3.12. Department Coordinator is a teacher nominated by a Department Council to co-ordinate the In-Semester examination of the PG programme in that department.

3.13. Faculty Advisor means a teacher from the parent department nominated by the Department Council, who will advise the students of a class on academic matters.

3.14. Course Teacher means a teacher who is in charge of a course. If a course is taught by more than one teacher, one teacher should be assigned as course teacher, nominated by the HOD. The course teacher shall be responsible for the valuation of answer scripts of examinations and other continuous assessments.

3.15. In-Semester Assessment (ISA) means assessment consisting of Attendance, Assignment/Seminar/Viva voce and Examination (theory and practical).

3.16. End Semester Assessment (ESA) means Examination conducted at the end of each semester for all courses (theory and practical).

3.17. Internal Examiner means a teacher working in the college.

3.18. External Examiner means a teacher from outside the college.

3.19. Grace Marks shall be awarded to candidates as per the orders issued by Mahatma Gandhi University.

3.20. Grade means a letter symbol (A, B, C, etc.), which indicates the broad level of performance of a student in a Course/ Semester/Programme.

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

3.22. College Average (CA) means average mark secured (ISA+ESA) for a course at the college level.

3.23. Words and expressions used and not defined in this regulation shall have the same meaning assigned to them in the Act and Statutes of the University, UGC Regulations and the Constitution of the CMS College Kottayam (Autonomous).

4. ELIGIBILITY FOR ADMISSION AND RESERVATION OF SEATS

Eligibility for admission, norms for admission and reservation of seats for various Postgraduate Programmes shall be according to the regulations framed/orders issued by Govt. of Kerala, Mahatma Gandhi University and CMS College Kottayam in this regard.

5. PROGRAMME STRUCTURE

5.1 The nomenclature of all PG programmes shall be as per the specifications of University Grants Commission and the Mahatma Gandhi University.

5.2 Credit Semester System (CSS) will be followed for all PG Programmes from the academic year 2019– 2020.

5.3 All the PG Programmes will be of two-year duration with four Semesters. A student may be permitted to complete the Programme, on valid reasons, within a period of 8 continuous semesters from the date of commencement of the first semester of the programme.

5.4 There will be three/four/five courses in each semester and one viva voce and dissertation at the end of the fourth semester.

5.5 There will be three components for the programme viz. core course, elective course and project spread over four semesters.

5.6 The total credits required for completing a PG Programme is **80**.

5.7 The Syllabus for all courses in each semester has been divided into five modules based on certain thematic commonalities.

6. EVALUATION SYSTEM

i. The evaluation scheme for each course shall contain two parts:
   (a) In-Semester Assessment (ISA)
   (b) End-Semester Assessment (ESA)

ii. The proportion of ISA to ESA will be 1:3.

iii. The marks secured for each course shall be converted as grades. The grades for different semesters and overall programme are assigned based on the corresponding semester grade point average and cumulative grade point average respectively.

iv. A separate minimum of 40% is mandatory for both ISA and ESA to pass for every course.

6.1 EVALUATION OF THEORY COURSES

The marks allotted for theory courses in End-Semester Assessment shall be 120 and that for the In-Semester Assessment will be 40.

A. IN-SEMESTER ASSESSMENT

The In-semester assessment for theory is based on the marks obtained for , Assignment, Major Seminar and two Test Papers for a particular course.

(i) Attendance

Percentage of attendance	Mark
90 and above	6
85 - 89	5
80 - 84	4
76 - 79	3
75	2
Below 75	0

Maximum marks = 6

(ii) Assignment (One assignment per course)

Evaluation Component	Mark
Review of related literature	2
Content	3
Reference	2
Punctuality	1

Maximum marks = 8

(iii) Major Seminar

A student should present one Major Seminar in a Semester. The faculty advisor should allot students to the respective course teacher in a semester. The seminar topics shall be incorporated in the syllabus for each course/ declared in the beginning of each semester. The student shall prepare the seminar paper with the guidance of the course teacher. The student is expected to make a detailed presentation in a common session in the department, with students and all course teachers. The student shall also make a brief conclusion including the future scope of studying the topic. The teacher in charge of the particular course has to act as the moderator for the seminar.

The course teachers of that semester shall evaluate the seminar and give marks for their course or the average mark of all the evaluators shall be taken as the seminar mark for each course of a semester.

Evaluation Component	Mark
Involvement/punctuality	1
Review of related literature	1
Content	3
Presentation	3
Interactions/ justification	1
Conclusion	1

Maximum marks = 10

(iv) Test paper

For each course, two In-Semester examinations of total 16 marks shall be conducted. One of the test paper will be centralized examination of 8 marks and the remaining 8 marks will be awarded with one or more class tests conducted by the course teacher.

B. END -SEMESTER ASSESSMENT

End-Semester examinations for each course are conducted at the end of every semester with a maximum marks of 120. The examination for each course will have two components viz., descriptive test and an objective type test. Questions shall be set to evaluate the attainment of course outcomes. The question paper for each course will be generated from the Question Bank which is prepared by due mapping of Course outcomes and Program Specific Outcomes.

(i) Descriptive Test

A written examination with a maximum marks of 100 and of three hours duration will be conducted.

PATTERN OF QUESTIONS

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

No.	Section	Type of questions	Total Questions	Number of questions to be answered	Mark for each question	Total Marks
1	Section A	Short answer type	8	5	4	20
2	Section B (One pair should be from each module)	Short essay/problem solving type	10 (Either/or)	5	8	40
3	Section C	Long essay type	4	2	20	40
	Total		**22**	**12**	-	**100**

(ii) Objective Test

A Multiple Choice Objective type Test shall be a component of the End-semester examination which will be conducted in the online mode for each course. The marks obtained shall be converted into 20. The objective type examination for all courses in a semester shall be conducted in a session of one hour. The number of questions in Arts stream will be 50 and that of Science and Mathematics stream will be 40.Questions should be equally distributed among the courses in a semester. There will be four choices for each question. Each question carries 4 marks for correct answer, zero marks for no answer and -1 marks for wrong answer.

6.2 EVALUATION OF PRACTICAL COURSES

Practical examination will be conducted at the end of each semester/ end of an academic year. The time of conduct of the practical examination will be decided by the respective BOS.

A. **IN-SEMESTER ASSESSMENT**

Evaluation Component	Mark
Attendance	6
Lab Involvement	8
Test	12
Record	8
Viva	6

Maximum Marks = 40

The components and the marks can be modified by the concerned BOS/Expert committee within the limit of maximum marks.

B. **END- SEMESTER ASSESSMENT**

Evaluation Component	Mark
Attendance	18
Lab Involvement	24
Test	36
Record	24
Viva	18

Maximum Marks = 120

The components and the marks can be modified by the concerned BOS/Expert committee within the limit of maximum marks.

6.3 EVALUATION OF PROJECT

An academic project work shall be done and a dissertation shall be submitted in the final semester of the programme. There will be both In semester and End semester assessment for the project work.

A. **IN- SEMESTER ASSESSMENT**

Evaluation Component	Mark
Relevance of the topic	5
Project content and report	15
Presentation	15
Project viva	10
Paper presentation* in Seminar/Conference or publications with ISBN/ISSN (*valid certificate to be submitted)	5

Maximum marks = 50

The components and the marks can be modified by the concerned BOS/Expert committee within the limit of maximum marks.

B. **END -SEMESTER ASSESSMENT**

The dissertation at the end of final Semester will be evaluated by a panel of one internal evaluator assigned by HOD and one external evaluator / a panel of two external evaluators, as may be decided by the respective BOS.

Evaluation Component	**Mark**
Relevance of the topic	15
Project content and report	45
Presentation	45
Project viva	30
Paper presentation* in Seminar/Conference or publications with ISBN/ISSN (*valid certificate to be submitted)	15

Maximum marks = 150

The components and the marks can be modified by the concerned BOS/Expert committee within the limit of maximum marks.

6.4 EVALUATION OF COMPREHENSIVE VIVA VOCE

A comprehensive viva voce shall be done at the end of the final semester. There will be both In-semester and End-semester assessment for the viva voce examination.

A. IN - SEMESTER ASSESSMENT

Evaluation Component	**Mark**
+2/ UG level questions	4
PG syllabus level questions	10
Subject of interest based questions	8
Advanced level questions	3

Maximum marks = 25

The components and the marks can be modified by the concerned BOS/Expert committee within the limit of maximum marks.

B. END- SEMESTER ASSESSMENT

The comprehensive Viva Voce Examination at the end of final Semester will be evaluated by a panel of one internal evaluator assigned by HOD and one external evaluator / a panel of two external evaluators, as may be decided by the respective BOS.

Evaluation Component	**Mark**
+2/ UG level questions	12
PG syllabus level questions	30
Subject of interest based questions	24
Advanced level questions	9

Maximum marks = 75

The components and the marks can be modified by the concerned BOS/Expert committee within the limit of maximum marks.

7. **Grievance Redressal Mechanism**

In order to address the grievance of students regarding In-Semester assessment, a two-level Grievance Redressal mechanism is established.

Level 1: Department Level: The Department cell is chaired by the HOD, Department Coordinator as member secretary and Course teacher in-charge as member. If the grievance is not redressed at the Department level, the student shall report the grievance to the College Level Grievance Redressal Cell.

Level 2: **College level**: College Level Grievance Redressal Cell has the Vice-Principal as the Chairman, Dean of Student Affairs as the Member Secretary and HOD of concerned Department as member.

8. **Eligibility for End Semester Examination**

A minimum of 75% average attendance for all the courses is mandatory to register for the examination. Condonation of shortage of attendance to a maximum of 10 days in a semester subject to a maximum of 2 times during the whole period of the programme may be granted by the College on valid grounds. Attendance may be granted to students attending University/College union/Co-curricular activities for the days of absence, on production of participation/attendance certificates, within one week, from the teacher in charge of the activity and endorsed by the Dean of Student Affairs. This is limited to a maximum of 10 days per semester. Monthly Attendance report will be published in the college website on or before the 10^{th} of every month. Those students who are not eligible even with condonation of shortage of attendance shall repeat the semester along with the next batch after obtaining readmission.

9. **Promotion to the next Semester**

Those students who possess the required minimum attendance and have registered for the End Semester Examination during an academic semester are promoted to the next semester.

Those students who possess the required minimum attendance and progress during an academic semester and could not register for the semester examination are permitted to apply for Notional Registration to the examinations concerned enabling them to get promoted to the next semester.

10. **Eligibility for Readmissions**

An additional chance of readmission will be given to those students who could not register for the examination due to shortage of attendance. Readmitted students shall continue their studies with the subsequent batch of students. If an applicant for readmission is found to have indulged in ragging or any other misconduct in the past, readmissions shall be denied.

11. **MARK CUM GRADE CARD**

The College under its seal shall issue to the student a MARK CUM GRADE CARD on completion of each semester/programme, which shall contain the following information:

(a) Name of the College
(b) Title of the Postgraduate Programme

(c) Name of the Semester
(d) Name and Register Number of the student
(e) Date of publication of result
(f) Code, Title, Credits and Maximum Marks (ISA, ESA & Total) of each course opted in the semester.
(g) ISA, ESA and Total Marks awarded, Grade, Grade point and Credit point in each course opted in the semester
(h) College average (CA) of the marks of all courses
(i) The total credits, total marks (Maximum & Awarded) and total credit points in the semester
(j) Semester Grade Point Average (SGPA) and corresponding Grade.
(k) Cumulative Grade Point Average (CGPA) and corresponding Grade.

The final Mark cum Grade Card issued at the end of the final semester shall contain the details of all courses taken during the study programme and the overall mark/grade for the total programme.

There shall be a College Level Monitoring Committee comprising Principal, Vice Principal as member-secretary, Dean of Academic Affairs, Controller of Examinations, IQAC Director and Administrative Assistant as members for the successful conduct of the scheme.

12. CREDIT POINT AND CREDIT POINT AVERAGE

Credit Point (CP) of a course is calculated using the formula:-
CP = C × GP, where C is the Credit and GP is the Grade point

Semester Grade Point Average (SGPA) of a Semester is calculated using the formula:-
SGPA = TCP/TC, where TCP is the Total Credit Point of that semester, ie, $\sum_1^n \mathrm{CPi}$; *TC is the Total Credit of that semester ie,* $\sum_1^n \mathrm{Ci}$, *where n is the number of courses in that semester*

Cumulative Grade Point Average (CGPA) is calculated using the formula:-
CGPA = TCP/TC, where TCP is the Total Credit Point of that programme ie, $\sum_1^n \mathrm{CPi}$; *TC is the Total Credit of that programme, ie,* $\sum_1^n \mathrm{Ci}$, *where n is the number of courses in that programme*

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Grades for the different courses, semesters and overall programme are given based on the corresponding CPA as shown below:

CPA	Grade with Indicator
4.5 to 5.0	A+ Outstanding
4.0 to 4.49	A Excellent
3.5 to 3.99	B+ Very Good
3.0 to 3.49	B Good (Average)
2.5 to 2.99	C+ Fair
2.0 to 2.49	C Marginal
Up to 1.99	D Deficient (Fail)

13. TRANSITORY PROVISION

Notwithstanding anything contained in these regulations, the Principal shall, for a period of six months from the date of coming into force of these regulations, have the power to provide by order that these regulations shall be applied to any programme with such modifications as may be necessary.

The Principal is also authorized to issue orders for the perfect realization of the regulations.

Annexure I

(Model Mark Cum Grade Card)

CMS COLLEGE KOTTAYAM (AUTONOMOUS)

Affiliated to Mahatma Gandhi University Kottayam

(Autonomous College as per UGC order no.F.22-1/216(AC)dated 9th March 2016)

MARK CUM GRADE CARD

Section	:	
Name of the Candidate	:	
Unique Permanent Registration Number	:	
Degree	:	
Programme	:	
Stream	:	
Name of the Examination	:	
Date of Publication of Result	:	

Course Code	Course Title	Credits (c)	Marks						Grade Awarded (G)	Grade Point (GP)	Credit Point (C x	College Average	Result
			ISA		ESA		TOTAL						
			Awarded	Maximum	Awarded	Maximum	Awarded	Maximum					

ISA - In - Semester Assessment, ESA – End - Semester Assessment

SGPA: **SG:**

Checked by **Section Officer** **Controller of Examinations**

Date:

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Annexure II

CMS COLLEGE KOTTAYAM (AUTONOMOUS)
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Affiliated to Mahatma Gandhi University Kottayam, Kerala
(Autonomous College as per UGC Order No.F.22-1/216 (AC) dated 9th March 2016)

CONSOLIDATED MARK CUM GRADE CARD

Name of the Candidate:

Unique Permanent Register Number (UPRN):

Degree:

Programme:

Stream:

Date of Birth:

Date of Eligibility for the Degree:

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CMS COLLEGE KOTTAYAM (AUTONOMOUS)

Name: UPRN:

Course Code	Course Title	Credits (C)	Marks						Grade Awarded (G)	Grade Point	Credit Point (CxGP)	College Average (CA)	Result
			ESA		ISA		Total						
			Awarded	Maximum	Awarded	Maximum	Awarded	Maximum					

Final Result

Cumulative Grade Point Average CGPA :

Semester Summary

Sl.No	Semester	Credit	SGPA	Grade	Month/year	Result
	Semester 1 Semester 2 Semester 3 Semester 4					

Date: **Controller of Examinations**

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Annexure III

(Reverse side of the Mark cum Grade Card (COMMON TO ALL SEMESTERS))

Description of the Evaluation Process

Grade and Grade Point

The Evaluation of each Course comprises of Internal and External Components in the ratio 1:3 for all Courses.

Grades and Grade Points are given based on the percentage of Total Marks (Internal + External) as given in Table 1

(Decimals are to be rounded mathematically to the nearest whole number)

Table 1

% Marks	Grade	GP
Equal to 88 and above	A+ Outstanding	5
Equal to 76 and < 88	A Excellent	4
Equal to64 and < 76	B+ Very Good	3
Equal to 52 and < 64	B Good(Average)	2
Equal to 40 and below 52	C Marginal	1
Below 40	D Deficient (Fail)	0
	Ab Absent	

Credit point and Credit point average

Grades for the different Semesters and overall Programme are given on a 7-point Scale based on the corresponding CPA, as shown in Table 2.

Credit point (**CP**) of a paper is calculated using the formula $\boldsymbol{CP = C \times GP}$**,where C is the Credit; GP is the Grade Point**

Semester or Programme (cumulative) Grade Point Average of a Course/Programme is calculated using the formula

SGPA/CGPA = $\boldsymbol{\frac{TCP}{TC}}$**, where TCP is the Total Credit Point; TC is the Total Credit**

Table 2

CPA	Grade with Indicator
4.5 to 5.0	A+ Outstanding
4.0 to 4.49	A Excellent
3.5 to 3.99	B+ Very Good
3.0 to 3.49	B Good (Average)
2.5 to 2.99	C+ Fair
2.0 to 2.49	C Marginal
Up to 1.99	D Deficient (Fail)

NOTE

A separate minimum of 40% marks each for internal and external (for both theory and practical) are required for a pass for a course. For a pass in a programme, a separate minimum of **Grade C** is required for all the individual courses. If a candidate secures **D Grade** for any one of the course offered in a Semester/Programme **only D grade** will be awarded for that Semester/Programme until he/she improves this to **C GRADE** or above within the permitted period.

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CURRICULUM

GRADUATE PROGRAMME OUTCOMES (GPO) – POST GRADUATE PROGRAMMES

At the completion of the Post Graduate Programme, the student will be able to accomplish the following programme outcomes.

GPO No.	Graduate Programme Outcomes
GPO.1	**Critical Thinking**: Ability to engage in independent and reflective thinking in order to understand logic connections between ideas.
GPO.2	**Effective Communication:** Development of communication skills for effectively transmitting and receiving information that focuses on acquiring knowledge, problem solving, improving on arguments and theories thereby paving the way for better employability and entrepreneurship.
GPO.3	**Social Consciousness:** Acquire awareness towards gender, environment, sustainability, human values and professional ethics and understand the difference between acting, responding and reacting to various social issues.
GPO.4	**Multidisciplinary Approach:** Combining various academic disciplines and professional specializations to cross borders and redefine problems in order to explore solutions based on the new understanding of complex situations.
GPO.5	**Subject Knowledge:** Acquiring knowledge at a higher level that would help develop the necessary skills, fuel the desire to learn and contribute to the field of expertise thereby providing valuable insights into learning and professional networking with the aim of catering to the local, national and global developmental needs.
GPO.6	**Lifelong Learning**: Understanding the necessity of being a lifelong learner for personal enrichment, professional advancement and effective participation in social and political life in a rapidly changing world.

PROGRAMME SPECIFIC OUTCOMES

PSO No.	**Program Specific Outcomes** Upon completion of this programme, the students will be able to,	**GPO No**
PSO1	Demonstrate advanced knowledge of fundamental principles of Chemistry in the core areas of Organic, Inorganic, Physical and Theoretical Chemistry.	1, 2,4,5
PSO2	Demonstrate advanced knowledge in multiple current areas of chemistry research such as Computational Chemistry, Spectroscopy, Organic Synthesis, Polymer Chemistry and Material Chemistry.	1,2,4,5,6
PSO3	Develop the knowledge of experimental techniques, theoretical concepts and acquire a broader understanding of research strategies, scientific thinking and data analysis	1,2,4,5
PSO4	Interpret research literature in his/her field of study and Conduct independent research under limited supervision within a research group and Communicate chemistry effectively, by using both oral and written skills.	1,2,3,4,5,6

PROGRAMME DESIGN

The Post graduate programme in Chemistry is a two year programme of four semesters. There are five components for the programme namely, the core course, elective course, practical course, viva-voce and a major project. In the first three semesters there are four core courses and three practical courses in each semester. In the fourth semester, there are three elective courses, three practical courses, a major project and a comprehensive viva-voce. The total credit for completing M.Sc. programme in Chemistry is 80.

The Course Design is given below:

Sl No	**COURSE TYPE**	**No. of courses**	**Total credits**
1.	Core courses	12	45
2.	Elective courses	3	12
3	Practical	6	18
4.	Viva –voce	2	2
5	Project	2	3
	TOTAL	**25**	**80**

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PROGRAMME STRUCTURE

	Code	Course	Hours/ Week	Total Hours	Credit
Semester 1	CH1921101	Organometallics and Catalysis	4	72	4
	CH1921102	Structural and Molecular Organic Chemistry	4	72	4
	CH1921103	Quantum Mechanics and Group Theory	4	72	4
	CH1921104	Classical and Statistical Thermodynamics	3	54	3
	CH1922601	Inorganic Chemistry Practical-I	3	54	Evaluation at the end of second semester
	CH1922602	Organic Chemistry Practical-I	3	54	
	CH1922603	Physical Chemistry Practical-I	4	72	
		Total	**25**	**450**	**15**
Semester 2	CH1922105	Coordination Chemistry	4	72	4
	CH1922106	Organic Reaction Mechanisms	4	72	4
	CH1922107	Chemical Bonding and Computational Chemistry	4	72	4
	CH1922108	Molecular Spectroscopy	3	54	3
	CH1922601	Inorganic Chemistry Practical-I	3	54	3
	CH1922602	Organic Chemistry Practical- I	3	54	3
	CH1922603	Physical Chemistry Practical-I	4	72	3
		Total	**25**	**450**	**24**
Semester 3	CH1923109	Structural Inorganic Chemistry	4	72	4
	CH1923110	Organic Syntheses	4	72	4
	CH1923111	Chemical Kinetics, Surface Chemistry and Photochemistry	4	72	4
	CH1923112	Spectroscopic Methods in Chemistry	3	54	3
	CH1924604	Inorganic Chemistry Practical- II	3	54	Evaluation at the end of fourth semester
	CH1924605	Organic Chemistry Practical- II	3	54	
	CH1924606	Physical Chemistry Practical- II	4	72	
		Total	**25**	**450**	**15**
Semester 4	CH1924301	Advanced Inorganic Chemistry(Elective)	5	90	4
	CH1924302	Advanced Organic Chemistry(Elective)	5	90	4
	CH1924303	Advanced Physical Chemistry(Elective)	5	90	4
	CH1924604	Inorganic Chemistry Practical- II	3	54	3
	CH1924605	Organic Chemistry Practical- II	3	54	3
	CH1924606	Physical Chemistry Practical-II	4	72	3
	CH1924801	Project			3
	CH1924901	Viva			2
		Total	**25**	**450**	**26**
Grand Total					**80**

DETAILED SYLLABUS OF ALL COURSES

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SEMESTER I

Course	Details				
Code	CH1921101				
Title	**ORGANOMETALLICS AND CATALYSIS**				
Degree	M.Sc.				
Branch(s)	Chemistry				
Year/Semester	1/I				
Type	Core Course				
Credits	4	**Hrs/Week**	4	**Total Hours**	72

CO No.	Expected Course Outcomes *Upon completion of this course, the students will be able to*:	Cognitive Level	PSO No.
1	Discuss the synthesis, structure and bonding in Organometallic compounds	E	1
2	Predict various carbonyl bonds in clusters	C	1
3	Differentiate different types of reactions of Organometallic compounds	An	1
4	Categorize compounds as isolobal and isoelectronic compounds	An	1
5	Describe catalysis by Organometallic compounds	U	1
6	Classify various bioinorganic compounds	Ap	1
7	Outline techniques and applications of nuclear chemistry	U	1

PSO – Programme Specific Outcome; CO-Course Outcome; Cognitive Level: R-Remember; U-Understanding; Ap-Apply; An-Analyze; E-Evaluate; C-Create.

Module	Course Description	Hrs	CO. No.
1.0	**Synthesis, Structure and Bonding of Organometallic Compounds**	**18**	**1, 2 &4**
1.1	Organometallic compounds with linear pi donor ligands-olefins, acetylenes,dienes and allyl complexes-synthesis, structure and bonding.	3	1
1.2	Complexes with cyclic pi donors-metallocenes and cyclic arene complexes**,**structure and bonding. Hapto nomenclature.	4	1
1.3	Carbene and carbyne complexes.	2	1
1.4	Preparation, properties, structure and bonding of simple mono and binuclear metal carbonyls, metal nitrosyls, metal cyanides and dinitrogen complexes.	4	1
1.5	Polynuclear metal carbonyls with and without bridging. Carbonyl clusters-LNCCS and HNCCS. IR spectral studies of bridging and non-bridging CO-ligands.	2	2
1.6	Isoelectronic and isolobal analogy	2	4
1.7	Wade-Mingos rules, cluster valence electrons	1	1

2.0	**Reactions of Organometallic Compounds**	**9**	**3**
2.1	Substitution reactions-nucleophilic ligand substitution, nucleophilic and electrophilic attack in coordinated ligands	3	3
2.2	Addition and elimination reactions-1,2 additions to double bonds, carbonylationand decarbonylation**,**Oxidative addition- concerted addition, SN2 reactions and radical and ionic mechanisms. Reductive elimination- binuclear reductive elimination and σ-bond metathesis. Oxidative coupling and reductive decoupling. Insertion (migration) and elimination reactions – insertions of CO and alkenes, insertion into M−H versus M−R and α, β, γ and δ eliminations.	5	3
2.3	Rearrangement reactions, redistribution reactions, fluxional isomerism.	1	
3.0	**Catalysis by Organometallic Compounds**	**18**	**5**
3.1	Homogeneous and heterogeneous organometallic catalysis-alkene hydrogenation using Wilkinson catalyst, Tolman catalytic loops.	1	5
3.2	Reactions of carbon monoxide and hydrogen-the water gas shift reaction, theFischer-Tropsch reaction (synthesis of gasoline). Hydroformylation of olefins using cobalt or rhodium catalyst.	2	5
3.3	Polymerization by organometallic initiators and templates for chain propagation Ziegler Natta catalysts. Polymerisation by metallocene catalysts.	2	5
3.4	Carbonylation reactions-Monsanto acetic acid process, carbonylation of butadiene using $Co_2(CO)_8$ catalyst in adipic ester synthesis. Carbonylation of alkenes and alkynes in the presence of a nucleophile: the Reppe reaction. Carbonylation of aryl halides in the presence of a nucleophile.	3	5
3.5	Olefin methathesis-synthesis gas based reactions. Photodehydrogenation catalyst (“Platinum Pop”).	2	5
3.6	Palladium catalysed oxidation of ethylene-the Wacker process. Epoxidation of olefins. Hydroxylation by metal-oxo complexes.	2	5
3.7	Asymmetric catalysis. Asymmetric hydrogenation, isomerisation and epoxidation.	2	5
3.8	C-H activation and functionalization of alkanes and arenes: Radical-type oxidation, hydroxylation, dehydrogenation, carbonylation and regioselectiveborylation of alkanes and cycloalkanes. Radical-type reactions, electrophilic reactions, carbonylation and borylation of arenes. Insertion of alkenes and alkynes in the Ar-H bond.	2	5
3.9	Application of palladium catalysts in the formation of C-O and C-N bonds. Oxidative coupling reactions of	2	5

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	alkynes with other unsaturated fragments for the formation of cyclic and heterocylic compounds. The Dotz reaction.		
4.0	**Bioinorganic Chemistry**	**18**	**6**
4.1	Essential and trace elements in biological systems. Structure and functions of biological membranes.	2	6
4.2	Mechanism of ion transport across membranes, sodium pump, ionophores, valinomycin and crown ether complexes of Na^+ and K^+. ATP and ADP.	3	6
4.3	Photosynthesis-chlorophyll a, PS I and PS II.	2	6
4.4	Role of calcium in muscle contraction, blood clotting mechanism and biological calcification.	1	6
4.5	Oxygen carriers and oxygen transport proteins-haemoglobins, myoglobins, cooperativity in haemoglobin, Bohr effect. Structure and functions of haemerythrins and haemocyanin.	3	6
4.6	Iron storage and transport in biological systems-ferritin and transferrin.	1	6
4.7	Redox metalloenzymes-cytochromes- cytochrome P450 and superoxide dismutase	2	6
4.8	Nonredox metalloenzymes-CarboxypeptidaseA-structure and functions. Nitrogen Fixation-nitrogenase. Vitamin B12 and the vitamin B12 coenzymes.	3	6
4.9	Metals in medicine-therapeutic applications of *cis*-platin, radio-isotopes and MRI agents. Toxic effects of metals(Cd, Hg, Cr and Pb)	1	6
5.0	**Nuclear Chemistry**	**9**	**7**
5.1	Radioactive decay- α, β and γ, nuclear isomerism & isomeric transition, internal conversion, Augerelectrons and Auger effect.	1	7
5.2	Nuclear Reactions- Q value and reaction threshold, reaction cross section, cross section and reaction rate, neutron capture cross section- variation of neutron capture cross section with energy (1/V law). Nuclear fission and fusion reactions- fission fragments and mass distribution, fission yields, fission energy, fission cross section and thresholf fission neutrons, nuclear fusion reactions and their applications.	2	7
5.3	Principles of counting technique such as G.M. counter, proportional, ionization and scintillation counters. Cloud chamber.	1	7
5.4	Synthesis of transuranic elements such as Neptunium, Plutonium, Curium, Berkelium, Einsteinium, Mendelevium, Nobelium, Lawrencium and elements with atomic numbers 104 to 109.	1	7
5.5	Analytical applications of radioisotopes-radiometric titrations, kinetics of exchange reactions, measurement of physical constants including diffusion constants,	2	7

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	Radioanalysis, Neutron Activation Analysis, Prompt Gama Neutron Activation Analysis and Neutron Absorptiometry.		
5.6	Applications of radio isotopes in industry, medicine, autoradiography,radiopharmacology, radiation safety precaution, nuclear waste disposal.Radiation chemistry of water and aqueous solutions.	1	7
5.7	Measurement of radiation doses. Relevance of radiation chemistry in biology,organic compounds and radiation polymerization.	1	7

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References:

1. J.E. Huheey, E.A. Keiter, R.L. Keiter, Inorganic Chemistry Principles of Structure and Reactivity, 4^{th}Edn., Harper Collins College Publishers,1993.
2. F.A. Cotton, G Wilkinson, C.A. Murillo, M. Bochmann, Advanced Inorganic Chemistry, 6th edition, Wiley-Interscience, 1999.
3. K.F. Purcell, J.C. Kotz, Inorganic Chemistry, Holt-Saunders, 1977.
4. P. Powell, Principles of Organometallic Chemistry, 2nd Edn., Chapman and Hall, 1988.
5. B.E. Douglas, D.H. McDaniel, J. J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Edn., Wiley-India, 2007.
6. B.D. Guptha, A.J Elias, Basic Organometallic Chemistry, Universities Press, 2010.
7. R.W. Hay, Bio Inorganic Chemistry, Ellis Horwood, 1984.
8. SumitBhaduri, DobleMukesh, Homogeneous Catalysis: Mechanism and Industrial Applications, Wiley Interscience, 2000.
9. Astruc, D.; Organometallic Chemistry and Catalysis, Springer Verlag, 2007.
10. Robert H. Crabtree, The Organometallic Chemistry of the Transition Metals, 4th Edn., Wiley Interscience, 2005.
11. R. M. Roat-Malone, Bioinorganic Chemistry A Short Course, Wiley Interscience, 2007.
12. Robert R. Crichton, Biological Inorganic Chemistry A New Introduction to Molecular Structure and Function, Elsevier, 2012.
13. H.J. Arnikar, Essentials of Nuclear Chemistry, Wiley Eastern, 1982.
14. S.N. Goshal, Nuclear Physics, S. Chand and Company, 2006.

Course	Details				
Code	CH1921102				
Title	**STRUCTURAL AND MOLECULAR ORGANIC CHEMISTRY**				
Degree	M.Sc.				
Branch(s)	Chemistry				
Year/Semester	1/I				
Type	Core Course				
Credits	4	**Hrs/Week**	4	**Total Hours**	72

CO No.	**Expected Course Outcomes** *Upon completion of this course, the students will be able to:*	Cognitive Level	PSO No.
1	To understand the basic concepts in organic chemistry	U	1
2	To describe and analyse the organic reactions by physical methods	An	1 2
3	To understand and analyse photochemical reactions	C	1
4	Understand and analyse reactions based on stereochemical aspects and applications	AP	2
5	To acquaint the student with conformational aspects	Ap	3

PSO – Programme Specific Outcome;CO-Course Outcome; Cognitive Level: R-Remember; U-Understanding; Ap-Apply; An-Analyze; E-Evaluate; C-Create.

Module	Course Description	Hrs	CO No.
1.0	**Basic Concepts in Organic Chemistry**	**18**	
1.1	Review of basic concepts in organic chemistry: Bonding, hybridisation, MO picture of butadiene and allyl systems.	2	1
1.2	Electron displacement effects: Inductive effect, electromeric effect, resonance effect, hyperconjugation, steric effect. Bonding weaker than covalent bonds.	3	1
1.3	Concept of aromaticity: Delocalization of electrons - Hückel's rule, criteria for aromaticity, examples of neutral and charged aromatic systems - annulenes. NMR as a tool ,carbon nanotubes and graphene	9	1
1.4	Mechanism of electrophilic and nucleophilic aromatic substitution reactions with examples. Arenium ion intermediates. SN1, SNAr, SRN1 and benzyne mechanisms	4	1
2.0	**Physical Organic Chemistry**	**9**	
2.1	Energy profiles. Kinetic versus thermodynamic control of product formation, Hammond postulate, kinetic isotope effects with examples. Linear free energy	5	2

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	relationships-Hammet equation, Taft equation		
2.2	Catalysis by acids,bases and nucleophiles with examples from acetal, cyanohydrin .Ester formation and hydrolysis reactions of esters-AAC2, AAC1, AAL1, BAC2and BAL1 mechanisms. Hard and soft acids, bases - HSAB principle and its applications (organic reactions only)	4	2
3.0	**Organic Photochemistry**	**9**	
3.1	Photoreactions of carbonyl compounds: Norrish reactions of ketones. Patterno-Buchi reaction. Barton (nitrite ester reaction); Di-π-methane and Photo Fries rearrangements, photochemistry of conjugated dienes (butadiene only),photochemistry of vision.	9	3
4.0	**Stereochemistry of Organic Compounds**	**18**	
4.1	Stereoisomerism: Definition based on symmetry and energy criteria, configuration and conformational stereoisomers,introduction to atrop isomerism	3	4
4.2	Center of chirality: Molecules with C, N, S based chiral centers, absolute configuration, enantiomers, racemic modifications, R and S nomenclature using Cahn-Ingold-Prelog rules, molecules with a chiral center and Cn, molecules with more than one center of chirality, definition of diastereoisomers, constitutionally symmetrical and unsymmetrical chiral molecules, erythro and threo nomenclature.	4	4
4.3	Axial, planar and helical chirality with examples, stereochemistry and absolute configuration of allenes, biphenyls and binaphthyls, ansa and cyclophanic compounds, spiranes, exo-cyclic alkylidene cycloalkanes.	4	4
4.4	Topicity and prostereoisomerism, topicity of ligands and faces as well as their nomenclature, NMR distinction of enantiotopic/diastereotopic ligands.	3	4
4.5	Geometrical isomerism: nomenclature, E-Z notation, methods of determination of geometrical isomers,interconversion of geometrical isomers	4	4
5.0	**Conformational Analysis**	**18**	
5.1	Conformational descriptors : Factors affecting conformational stability of molecules, conformational analysis of substituted ethanes, cyclohexane and its derivatives, decalins, adamantane, norbornane,sucrose and lactose.	6	5
5.2	Conformation and reactivity of elimination (dehalogenation, dehydrohalogenation, semipinacolic deamination and pyrolytic elimination - Saytzeff and Hofmann eliminations), substitution and oxidation of 2^o alcohols.	9	5
5.3	Chemical consequence of conformational equilibrium - Curtin Hammett principle.	3	5

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References:

1. R. Bruckner, Advanced Organic Chemistry: Reaction Mechanisms, Academic Press, 2002.
2. F.A. Carey, R.A. Sundberg, Advanced Organic Chemistry, Part A: Structure and Mechanisms, 5thEdn., Springer, 2007.
3. J. Clayden, N. Greeves, S. Warren, P. Wothers, Organic Chemistry, Oxford University Press, 2004.
4. T.H. Lowry, K.S. Richardson, Mechanism and Theory in Organic Chemistry, 2^{nd}Edn., Harper & Row, 1981.
5. N.S. Isaacs, Physical Organic Chemistry, ELBS/Longman, 1987.
6. D. Nasipuri, Stereochemistry of Organic Compounds: Principles and Applications, 3^{rd}Edn., New Age Pub., 2010.
7. D.G. Morris, Stereochemistry, RSC, 2001.
8. E.L. Eliel, S.H. Wilen, Stereochemistry of Organic Compounds, John Wiley & Sons, 1994.
9. N.J. Turro, V. Ramamurthy, J.C. Scaiano, Principles of Molecular Photochemistry: An Introduction, University Science books, 2009.
10. N.J. Turro, Modern Molecular Photochemistry, Benjamin Cummings, 1978.
11. K.K.R. Mukherjee, Fundamentals of Photochemistry, New Age Pub., 1978.
12. Jerry March, Advanced Organic Chemistry: Reactions, Mechanisms, and Structure
13. Nature Chemistry, Vol 10, 2018, pp 618 – 624

Course	Details				
Code	CH1921103				
Title	**QUANTUM MECHANICS AND GROUP THEORY**				
Degree	M.Sc.				
Branch(s)	Chemistry				
Year/Semester	1/I				
Type	Core Course				
Credits	4	**Hrs/Week**	4	**Total Hours**	72

CO No.	**Expected Course Outcomes** *Upon completion of this course, the students will be able to*:	Cognitive Level	PSO No.
1	Understand and Familiarize with the main aspects of the historical development of quantum mechanics and understand the central concepts and principles in quantum mechanics	U	1, 3
2	Solve the Schrödinger equation for simple systems in one to three dimensions	Ap	1, 3
3	Understand the concepts of angular momentum and spin, as well as the rules for quantization and addition of these.	Ap	1,3
4	Evaluate symmetry elements in a molecule and classify molecules into point groups and evaluate symmetry elements in a crystal and classify crystals into point groups	E	1, 3
5	Apply group theoretical rules to derive group multiplication tables, matrix representations, classes, character tables of point groups	Ap	1, 3
6	Apply group theory to analyze vibration, Raman spectra and electronic spectra of polyatomic molecules.	An	1, 3

PSO – Programme Specific Outcome; CO-Course Outcome; Cognitive Level: R-Remember; U-Understanding; Ap-Apply; An-Analyze; E-Evaluate; C-Create.

Module	Course Description	Hrs	CO. No.
1.0	**Foundation of Quantum Mechanics**	**9**	
1.1	Historical background: Blackbody Radiation, Photoelectric effect, Compton effect, Hydrogen atom spectra, Matter waves	2	**1**
1.2	Operators: Linear operators, eigen functions and eigen values, commutation and non-commutation, construction of operators, normalization concept, Hermitian operators.	3	**1**
1.3	Postulates of quantum mechanics, time-independent and time-dependent Schrödinger equation.	3	**1**
1.4	Evolution of states, Uncertainty principle, Characteristics of wavefunction	1	**1**
2.0	**Application of Schrödinger's Equations to Exactly**	**22**	

	Solvable Model Problems		
2.1	Translational motion: free particle in one-dimension.	2	**2**
2.2	Penetration into and through barriers: infinitely thick potential well, barrier of finite width	2	**2**
2.3	Particle in a box: one-dimensional box, particle in a three dimensional box- separation of variables, degeneracy.	4	**2**
2.4	Vibrational motion: one-dimensional harmonic oscillator (complete treatment), Hermite equation(solving by method of power series), Hermite polynomials, recursion relation, wave functions and energies	4	**2**
2.5	Rotational motion: Particle on a ring and its solution	2	**2**
2.6	Non-planar rigid rotor (or particle on a sphere) and their solutions, Legendre and associated Legendre equations, Legendre and associated Legendre polynomials. Spherical harmonics (imaginary and real forms)	4	**2**
2.7	Hydrogen-like Atoms: Schrodinger equation and its solutions, wave functions and energies of hydrogen-like atoms. Probabilities and radial distribution functions, atomic orbitals, degeneracy.	4	**2**
3.0	**Angular momentum**	**5**	
3.1	Quantization of angular momentum, quantum mechanical operators corresponding to angular momenta (Lx, Ly, Lz and L^2),	2	3
3.2	Commutation relations between these operators, shift operators, eigenvalues of angular momentum, Spin: Spin orbitals, construction of spin orbitals from orbitals and spin functions.	3	3
4.0	**Theory of Molecular Symmetry and Group Theory**	**27**	**4,5**
4.1	Symmetry elements, symmetry operations, point groups and their symbols, sub groups, classes, abelian and cyclic groups, group multiplication tables-classes in a group and similarity transformation.	5	4,5
4.2	Matrices: addition and multiplication of matrices, inverse and orthogonal matrices, character of a matrix, block diagonalization, matrix representation of symmetry operations, representation of groups by matrices, construction of representation using vectors and atomic orbitals as basis, representation generated by cartesian coordinates positioned on the atoms of a molecule (H_2O and SO_2 as examples).	10	5
4.3	Reducible and irreducible representations-construction of irreducible representation by standard reduction formula. Statement of Great Orthogonality Theorem (GOT). Properties of irreducible representations. Construction of irreducible representation using GOT-construction of character tables for C_{2v}, C_{2h}, C_2,C_{3v} and C_{4v}. Direct product of representations.	12	5
5.0	**Group theory in spectroscopy and crystallography**	**9**	
5.1	Applications in vibrational spectra: transition moment integral, vanishing of integrals, symmetry aspects of	4	6

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	molecular vibrations, vibrations of polyatomic molecules – selection rules for vibrational spectroscopy. Determination of the symmetry of normal modes of H_2O, Trans-N_2F_2 and NH_3 using Cartesian coordinates and internal coordinates. Complementary character of IR and Raman spectra-determination of the number of active IR and Raman lines.		
5.2	Application in electronic spectra: Selection rules for electronic transition, electronic transitions due to the carbonyl chromophore in formaldehyde.	2	6
5.3	Symmetry in crystals: 32 crystallographic point groups (no derivation), Hermann-Mauguin symbols. Screw axis-pitch and fold of screw axis. Glide planes. Space groups-determination of space group symbols of triclinic and monoclinic systems.	3	4

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Course texts:

1. P.W. Atkins, R.S. Friedman, Molecular Quantum Mechanics, 4th Edn., Oxford University Press, 2005.
2. F.A. Cotton, Chemical Applications of Group Theory, 3rd Edn., Wiley Eastern, 1990.
3. A.S. Kunju, G. Krishnan, Group Theory and its Applications in Chemistry, PHI Learning, 2010
4. R. Ameta, Symmetry and Group Theory in Chemistry, New Age International, 2013

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1. I.N. Levine, Quantum Chemistry, 6th Edn., Pearson Education Inc., 2009.
2. D.A. McQuarrie, Quantum Chemistry, University Science Books, 2008.
3. J.P. Lowe, K Peterson, Quantum Chemistry, 3rd Edn., Academic Press, 2006.
4. T. Engel, Quantum Chemistry and Spectroscopy, Pearson Education, 2006.
5. H. Metiu, Physical Chemistry:Quantum Mechanics, Taylor & Francis, 2006.
6. L. H. Hall, Group Theory and Symmetry in Chemistry, McGraw Hill,1969
7. V. Ramakrishnan, M.S. Gopinathan, Group Theory in Chemistry, Vishal Publications, 1992.
8. S. Swarnalakshmi, T. Saroja, R.M. Ezhilarasi, A Simple Approach to Group Theory in Chemistry, Universities Press, 2008.
9. S.F.A. Kettle, Symmetry and Structure: Readable Group Theory for Chemists, 3rd Edn., Wiley, 2007.
10. A. Vincent, Molecular Symmetry and Group Theory: A Programmed Introduction to Chemical Applications, 2nd Edn., Wiley, 2000.

Course	Details				
Code	CH1921104				
Title	**CLASSICAL AND STATISTICAL HERMODYNAMICS**				
Degree	M.Sc.				
Branch(s)	Chemistry				
Year/Semester	1/1				
Type	Core Course				
Credits	3	**Hrs/Week**	3	**Total Hours**	54

CO No.	**Expected Course Outcomes** *Upon completion of this course, the students will be able to:*	Cognitive Level	PSO No.
1	Understand the basic concepts of classical and statistical thermodynamics	U	1
2	Analyze the macroscopic properties of matter using classical and statistical thermodynamics	An	1, 3
3	Relate microscopic and macroscopic properties using classical and statistical thermodynamics	An	1, 3
4	Calculate change in thermodynamic properties and absolute values of thermodynamic quantities and equilibrium constants	Ap	1, 3
5	Understand the fundamental concepts of irreversible thermodynamics	U	1

PSO – Programme Specific Outcome; CO-Course Outcome; Cognitive Level: R-Remember; U-Understanding; Ap-Apply; An-Analyze; E-Evaluate; C-Create.

Module	Course Description	Hrs	CO No.
1.0	**Thermodynamics of ideal systems**	**9**	**1,2,3,4**
1.1	Brief review on the basic concepts in thermodynamics: First law of thermodynamics (work, heat, energy, internal energy, enthalpy: definition), State and path functions and their significance.	1	1,2,3
1.2	Second law of thermodynamics: Entropy (basic concept, definition) Clausius inequality, variation of entropy with T,P,V	3	1,2,4
1.3	Helhmotz energy, Gibbs energy, Criterion for spontaneity, Maxwell relations and its significance, Fundamental equations, variation of G with T&P(Gibbs Helmholtz equation, applications of Gibbs Helmholtz equation).	5	1,2,3
2.0	**Thermodynamics of non-ideal systems**	**16**	**1,2,4**
2.1	Partial molar quantities, chemical potential and Gibbs-Duhem equations, determination of partial molar volume and enthalpy.	3	1,2,4
2.2	Fugacity, relation between fugacity and pressure, determination of fugacity of a real gas, variation of	3	1,2,4

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	fugacity with temperature and pressure. Activity (solute, solvent, ideal dilute solution), dependence of activity on temperature and pressure.		
2.3	Thermodynamics of mixing (entropy of mixing &free energy of mixing), Margules relations, excess thermodynamic functions-free energy, enthalpy, entropy and volume. Determination of excess enthalpy and volume.	3	1,2,4
2.4	Chemical affinity and thermodynamic functions, equilibrium constant- for ideal gas, general equation, relation connecting K with various TD variables, effect of temperature and pressure on chemical equilibrium-Van Hoff equation.	4	1,2,4
2.5	Third law of thermodynamics, Nernst heat theorem, determination of absolute entropies using third law, entropy changes in chemical reactions.	3	1,2,4
3.0	**Irreversible thermodynamics**	**2**	**1,5**
3.1	Thermodynamics of irreversible processes with simple examples. Entropy production- rate of entropy production, entropy production in chemical reactions. The principle of microscopic reversibility, the Onsager reciprocal relations.	2	1,5
4.0	**Fundamentals of Statistical Mechanics**	**23**	**1,2,3,4**
4.1	Mathematical Preliminaries: Basic probability theory: fundamentalcounting principle, permutations, configurations, binomial probabilities, Stirling's approximation	3	1,2,3
4.2	Probability distribution functions, Probability distribution involving discrete and continuous variable, Characterizing distribution functions: Average value, distribution moments, variance.	4	1,2,3,4
4.3	Boltzmann distribution: microstates and configuration, Derivation of Boltzmann distribution, Physical meaning of the Boltzmann distribution law, Definition of beta.	3	1,2,3
4.4	Ensemble: Canonical ensemble, relating q to Q for an ideal gas, translation partition function, rotational partition function: diatomic and polyatomic, Vibrational partition function, equi-partition theorem, Electronic partition function.	4	1,2,3
4.5	Thermodynamic information in the partition function: Energy, heat capacity, entropy, Helmholtz energy, enthalpy, Gibbs energy	4	1,2,3
4.6	Quantum statistics: Indistinguishable particles and quantum statistics, Bose-Einstein statistics, Fermi-Dirac statistics.	2	1,2,3
4.7	Fundamental concepts and Postulates of statistical mechanics: Phase space and trajectory, Time average equals ensemble average, equal a priori	3	1,2,3

	probability, ergodic hypothesis, measure of ergodicity, Lioville theorem and lioville equation, phase space density, Hamilton's equation of motion		
5.0	**Computer simulation methods in statistical mechanics**	**4**	**1,2,3**
5.1	Monte Carlo simulations: Importance sampling, Metropolis method	2	1,2,3
5.2	Molecular Dynamics simulations: Force calculation, Integrating equations of motion: Verlet algorithm, Velocity Verlet algorithm	2	1,2,3

Course Texts:

1. P.W. Atkins, Physical Chemistry, Oxford University press, 8^{th} edition
2. Thomas Engel and Philip Reid, Thermodynamics, Statistical Thermodynamics &Kinetics, Pearson (4^{th} Edition), 2018
3. Mark Tuckerman, Statistical Mechanics: Theory and Molecular Simulation, Oxford university Press, 2010.

References:

1. A. M Glazer, J. S Wark, Statistical Mechanics: A survival guide, Oxford University Press (1^{st} edition), 2001.
2. J. Rajaram, J.C. Kuriakose, Thermodynamics, S Chand and Co., 1999.
3. K.J. Laidler, J.H. Meiser, B.C. Sanctuary, Physical Chemistry, 4th Edn., Houghton Mifflin, 2003.
4. L.K. Nash, Elements of Classical and Statistical Mechanics, 2nd Edn., Addison Wesley, 1972.
5. D.A. McQuarrie, J.D. Simon, Physical Chemistry: A Molecular Approach, University Science Books,1997
6. C. Kalidas, M.V. Sangaranarayanan, Non-equilibrium Thermodynamics, Macmillan India, 2002.
7. R.K. Murray, D.K. Granner, P. A. Mayes, V.W. Rodwell, Harper's Biochemistry, Tata McGraw Hill,1999.
8. Tinoco, K. Sauer, J.C. Wang, J.D. Puglisi, Physical Chemistry: Principles and Applications in Biological Science, Prentice Hall,2002
9. F.W. Sears, G.L. Salinger, Thermodynamics, Kinetic Theory and Statistical Thermodynamics, Addison Wesley, 1975.
10. J. Kestin, J.R. Dorfman, A Course in Statistical Thermodynamics, Academic Press, 1971.

Course	Details				
Code	CH1922601				
Title	**INORGANIC CHEMISTRY PRACTICAL-I**				
Degree	M.Sc.				
Branch(s)	Chemistry				
Year/Semester	1/ I&II				
Type	Practical				
Credits	3	**Hrs/Week**	3	**Total Hours**	54

CO No.	**Expected Course Outcomes** *Upon completion of this course, the students will be able to:*	Cognitive Level	PSO No.
1	To identify and differentiate between the different rare earth cations by different analytical methods.	U	1,3
2	Develop advanced laboratory skills used in inorganic synthesis including spectroscopic and analytical techniques for identification and characterization of inorganic molecules.	Ap	2
3	Application of safety and chemical hygiene regulations and practices.	Ap	3

PSO – Programme Specific Outcome; CO-Course Outcome; Cognitive Level: R-Remember; U-Understanding; Ap-Apply; An-Analyze; E-Evaluate; C-Create.

Module	Course Description	Hrs	CO No.
1.0	**Separation and identification of two less familiar metal ions**	**54**	
1.1	Separation and identification of two less familiar metal ions such as Tl, W, Se, Mo, Ce, Th, Ti, Zr, V, U and Li. (Anions which need elimination not to be given. Minimum eight mixtures to be given.)	54	1,2,3
2.0	**Colorimetric estimation of metal ions**	**27**	
2.1	Colorimetric estimation of Fe, Cu, Ni, Mn, Cr, NH_4^+, nitrate and phosphate ions.	27	1,2,3
3.0	**Preparation and characterization of metal complexes**	**27**	
3.1	Preparation and characterization ofcomplexes using IR, NMR and electronic spectra. (a) Tris (thiourea)copper(I) complex (b) Potassium tris (oxalato) aluminate (III). (c) Hexammine cobalt (III) chloride. (d) Tetrammine copper (II) sulphate. (e) Schiff's base complexes of various divalent metal ions.	27	1,2,3

References:

1. A.I. Vogel, G.Svehla,;Vogel's Qualitative Inorganic Analysis, 7th Edn., Longman,1996.
2. A.I. Vogel, A Text Book of Quantitative Inorganic Analysis, Longman,1966.
3. I.M. Koltoff, E.B. Sandell, Text Book of Quantitative Inorganic Analysis, 3rd Edn.,McMillian, 1968.
4. V.V. Ramanujam, InorganicSemimicro Qualitative Analysis, The NationalPub.Co.,1974.

Course	Details				
Code	CH1922602				
Title	**ORGANIC CHEMISTRY PRACTICAL-I**				
Degree	M.Sc.				
Branch(s)	Chemistry				
Year/Semester	1/I&II				
Type	Practical				
Credits	3	**Hrs/Week**	3	**Total Hours**	54

CO No.	**Expected Course Outcomes** *Upon completion of this course, the students will be able to*:	Cognitive Level	PSO No.
1	Qualitatively separate the organic components	An	3
2	Provide hands on experience in the preparation of TLC, column chromatography	An	3
3	Develop skills in separating techniques	C	3
4	Acquire advanced knowledge in chemical drawing	C	4

PSO – Programme Specific Outcome; CO-Course Outcome; Cognitive Level: R-Remember; U-Understanding; Ap-Apply; An-Analyze; E-Evaluate; C-Create.

Module	Course Description	Hrs	CO No.
1.0	**PART I**	**27**	
1.1	General methods of separation and purification of organic compounds such as: Solvent extraction Soxhlet extraction Fractional crystallization TLC and Paper Chromatography Column Chromatography Membrane Dialysis	27	1,4
2.0	**PART II**	**54**	
2.1	Separation of Organic binary mixtures by chemical/solvent separation methods	18	3,4
2.2	Separation of organic mixtures by TLC	12	3,4
2.3	Separation/ purification of organic mixtures by column chromatography	14	3,4
2.4	Test for detection of rosin in soaps. Estimation of rosin in soaps	10	3,4
3.0	**PART III**	**27**	
3.1	Drawing the structures of organic molecules and reaction schemes by ChemDraw, Symyx Draw and Chemsketch.	18	1,4
3.2	Draw the structures and generate the IR and NMR spectra of the substrates and	9	1,4

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	products in the following reactions: 1. Cycloaddition of diene and dienophile (Diels-Alder reaction) 2. Oxidation of primary alcohol to aldehyde and then to acid 3. Benzoin condensation 4. Esterification of simple carboxylic acids 5. Aldol condensation		

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References:

01. A.I. Vogel, A Textbook of Practical Organic Chemistry, Longman, 1974.
02. A.I. Vogel, Elementary Practical Organic Chemistry, Longman, 1958.
03. F.G. Mann, B.C Saunders, Practical Organic Chemistry, 4th Edn., Pearson Education, India, 2009.
04. R. Adams, J.R. Johnson, J.F. Wilcox, Laboratory Experiments in OrganicChemistry, Macmillan, 1979.

Course	Details				
Code	CH1922603				
Title	**PHYSICAL CHEMISTRY- PRACTICAL – I**				
Degree	M.Sc.				
Branch(s)	Chemistry				
Year/Semester	1/I & II				
Type	Practical				
Credits	3	Hrs/Week	4	Total Hours	72

CO No.	**Expected Course Outcomes** *Upon completion of this course, the students will be able to:*	Cognitive Level	PSO No.
1	Interpret data from various experiments, including the construction of appropriate graphs and evaluation of errors.	An	3, 4
2	Quantitatively analyze the extent of adsorption of liquids by solids.	An	1
3	Understand the concept of surface forces in various liquids and the effect of reaction conditions on it.	An	3
4	Apply the terms of phase diagrams in binary and tertiary systems which are used in material science and engineering field.	Ap	1
5	Develop skills in applying the distribution law for various solutes between different appropriate solvent pairs in liquid phase chemical reactions.	C	3
6	Compare and apply theoretical approaches such as HF, MP2, DFT in stimulating various scientific problems and calculating various properties of molecules using Gaussian 09 Quantum Chemistry program	C	3

PSO – Programme Specific Outcome; CO-Course Outcome; Cognitive Level: R-Remember; U-Understanding; Ap-Apply; An-Analyze; E-Evaluate; C-Create.

Module	Course Description	Hrs	CO No.
1.0	**Adsorption**	**12**	**1,2**
1.1	Verification of Freundlich and Langmuir adsorption isotherm: charcoal-acetic acid or charcoal-oxalic acid system.	6	1,2
1.2	Determination of the concentration of the given acid using the isotherms.	6	1,2
2.0	**Surface tension**	**18**	**1,3**
2.1	Determination of the surface tension of a liquid by a) Capillary rise method b) Drop number method c) Drop weight method	6	1,3
2.2	Determination of parachor values.	6	1,3
2.3	Determination of the composition of two liquids by	6	1,3

	surface tension measurements		
3.0	**Phase diagrams**	**24**	**1,4**
3.1	Construction of phase diagrams of simple eutectics.	6	1,4
3.2	Construction of phase diagram of compounds with congruent melting point: diphenyl amine-benzophenone system.	6	1,4
3.3	Effect of (KCl/succinic acid) on miscibility temperature.	6	1,4
3.4	Construction of phase diagrams of three component systems with one pair of partially miscible liquids.	6	1,4
4.0	**Distribution Law**	**18**	**1,5**
4.1	Distribution coefficient of iodine between an organic solvent and water.	6	1,5
4.2	Distribution coefficient of benzoic acid between benzene and water	6	1,5
4.3	Determination of the equilibrium constant of the reaction $KI + I_2 \leftrightarrow KI_3$	6	1,5
5.0	**Computational chemistry experiments**	**72**	**1,5**
5.1	Single point energy calculations	12	1,5
5.2	Geometry optimization calculations	12	1,5
5.3	3. Frequency calculations	12	1,5
5.4	Basis set effects	12	1,5
5.5	Predicting Ionization energy, electron affinity, proton affinity and atomization energies.	12	1,5
5.6	Studying chemical reactions and reactivity	12	1,5

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References:

1. J.B. Yadav, Advanced Practical Physical Chemistry, Goel Publishing House, 2001.
2. G.W. Garland, J.W. Nibler, D.P. Shoemaker, Experiments in Physical Chemistry, 8thEdn., McGraw Hill, 2009.
3. J.B. Yadav, Advanced Practical Physical Chemistry, Goel Publishing House, 2001.
4. G.W. Garland, J.W. Nibler, D.P. Shoemaker, Experiments in Physical Chemistry, 8th Edn., McGraw Hill, 2009.
5. James B. Foresman and Aeleen Frisch, Exploring Chemistry With Electronic Structure Methods: A Guide to Using Gaussian, Gaussian, second edition, 1996
6. Gaussian 09, Revision A.02, M. J. Frisch*et.al*, 2016.

SEMESTER II

Course	Details				
Code	CH1922105				
Title	**COORDINATION CHEMISTRY**				
Degree	M.Sc.				
Branch(s)	Chemistry				
Year/Semester	1/II				
Type	Core Course				
Credits	4	**Hrs/Week**	4	**Total Hours**	72

CO No.	**Expected Course Outcomes** *Upon completion of this course, the students will be able to*:	Cognitive Level	PSO No.
1	Classify various coordination compounds and sigma & pi bonding ligands	Ap	1
2	Explain different bonding aspects in coordination compounds	An	1
3	Investigate electronic, magnetic and spectral properties of coordination compounds	An	1
4	Propose structure to coordination compounds	C	1
5	Discuss the kinetics and mechanism of reactions of coordination compounds	E	1
6	Describe stereochemistry of coordination compounds	U	1
7	Summarize different properties of lanthanides and actinides	U	1
8	Compare the properties of coordination compounds of lanthanides and actinides	An	1

PSO – Programme Specific Outcome; CO-Course Outcome; Cognitive Level: R-Remember; U-Understanding; Ap-Apply; An-Analyze; E-Evaluate; C-Create.

Module	Course Description	Hrs	CO No.
1.0	**Structural Aspects and Bonding of Coordination compounds**	**18**	**1&2**
1.1	Classification of complexes based on coordination numbers and possible geometries.	2	1
1.2	Sigma and pi bonding ligands such as CO, NO, CN-, R_3P, and Ar_3P.	2	1
1.3	Stability of complexes, thermodynamic aspects of complex formation-Irving William order of stability, chelate effect.	2	2
1.4	Splitting of *d* orbitals in octahedral, tetrahedral, square planar, square pyramidal and triagonal bipyramidal fields, LFSE, *Dq* values.	4	2
1.5	Jahn Teller (JT) effect.	2	2
1.6	Theoretical failure of crystal field theory, evidence of	2	2

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	covalency in the metalligand bond, nephelauxetic effect, ligand field theory.		
1.7	Molecular orbital theory M.O energy level diagrams for octahedral and tetrahedral complexes without and with π-bonding, experimental evidences for pi-bonding.	4	2
2.0	**Spectral and Magnetic Properties of Metal Complexes**	**18**	**3&4**
2.1	Electronic Spectra of complexes-Term symbols of d^nsystem, Racah parameters, splitting of terms in weak and strong octahedral and tetrahedral fields.	2	3
2.2	Correlation diagrams for d^n and d^{10-n}ions in octahedral and tetrahedral fields (qualitative approach).	2	3
2.3	*d-d* transition, selection rules for electronic transition-effect of spin orbit coupling and vibronic coupling.	2	3
2.4	Interpretation of electronic spectra of complexes-Orgel diagrams, demerits of Orgel diagrams	2	3
2.5	Tanabe-Sugano diagrams, calculation of *Dq*, *B* and β (Nephelauxetic ratio) values	2	3
2.6	Spectra of complexes with lower symmetries. Charge transfer spectra, luminescence spectra	3	3
2.7	Magnetic properties of complexes-paramagnetic and diamagnetic complexes, molar susceptibility, Gouy method for the determination of magnetic moment of complexes, spin only magnetic moment.	2	3
2.8	Temperature dependence of magnetism Curie's law, Curie-Weiss law. Temperature Independent Paramagnetism (TIP) Spin state cross over, Antiferromagnetism-inter and intramolecular interaction. Anomalous magnetic moments.	2	3
2.9	Elucidating the structure of metal complexes (cobalt and nickel complexes) usingelectronic spectra, IR spectra and magnetic moments.	1	4
3.0	**Kinetics and Mechanism of Reactions in Metal Complexes**	**18**	**5**
3.1	Thermodynamic and kinetic stability, kinetics and mechanism of nucleophilicsubstitution reactions in square planar complexes	4	5
3.2	*Trans*-effect-theory and applications**.** Effect of entering ligand, effect of leaving group and effect of ligands already present on reaction rate, effect of solvent and reaction pathways. Substitution in tetrahedral and five-coordinate complexes.	2	5
3.3	Kinetics and mechanism of octahedral substitution- water exchange, dissociative and associative mechanisms.	4	5
3.4	Base hydrolysis, racemization reactions, solvolytic reactions (acidic and basic). Replacement reactions involving multidendate ligands- The formation of chelates, effect of H+ on the rates of substitution of chelate complexes, metal ion assisted and ligand assisted dechelation.	4	5
3.5	Electron transfer reactions: outer sphere mechanism-Marcus theory, inner sphere mechanism-Taube mechanism. Mixed	4	5

	outer and inner sphere reactions. Two electron transfer and intramolecular electron transfer.		
4.0	**Stereochemistry of Coordination Compounds**	**9**	**6**
4.1	Geometrical and optical isomerism in octahedral complexes,	2	6
4.2	Resolution of optically active complexes, determination of absolute configuration of complexes by ORD and circular dichroism, stereoselectivity and conformation of chelate rings.	3	6
4.3	Asymmetric synthesis catalyzed by coordination compounds.	1	6
4.4	Linkage isomerism-electronic and steric factors affecting linkage isomerism.	1	6
4.5	Symbiosis-hard and soft ligands, Prussian blue and related structures. Macrocycles-crown ethers.	2	6
5.0	**Coordination Chemistry of Lanthanides and Actinides**	**9**	**7&8**
5.1	General characteristics of lanthanides-Electronic configuration, Term symbols forlanthanide ions, Oxidation state, Lanthanide contractio**n.** Organometallic complexes of the lanthanoids- σ-bonded complexes, cyclopentadienyl complexes, organolanthanoid complexes as catalysts.	1	7
5.2	Factors that mitigateagainst the formation of lanthanide complexes.	1	7
5.3	Electronic spectra and magneticproperties of lanthanide complexes.	1	7
5.4	Lanthanide complexes as shift reagents.	1	7
5.5	General characteristics of actinides-difference between ***4f***and ***5f***orbitals. Coordination complexes of the actinoids-sandwich complexes, coordination complexes and organometallic compounds of thorium and uranium.	2	8
5.6	Comparative account of coordination chemistry of lanthanides and actinides with special reference to electronic spectra and magnetic properties.	3	8

References:

1. F.A. Cotton, G. Wilkinson, Advanced Inorganic Chemistry: A Comprehensive Text, 3rd Edn., Interscience,1972.
2. J.E. Huheey, E.A. Keiter, R.A. Keiter, Inorganic Chemistry Principles of Structure and Reactivity, 4thEdn., Pearson Education India, 2006.
3. K.F. Purcell, J.C. Kotz, Inorganic Chemistry, Holt-Saunders, 1977.
4. F. Basolo, R.G. Pearson, Mechanisms of Inorganic Reaction, John Wiley & Sons, 2006.
5. B.E. Douglas, D.H. McDaniel, J.J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd Edn., Wiley-India, 2007.
6. R.S. Drago, Physical Methods in Chemistry, Saunders College, 1992.
7. B.N. Figgis, M.A. Hitchman, Ligand Field Theory and its Applications, Wiley-India, 2010.
8. J.D. Lee, Concise Inorganic Chemistry, 4th Edn., Wiley-India, 2008
9. R. G. Wilkins, Kinetics and Mechanisms of Reactions of Transition Metal Complexes, Wiley VCH, 2002.
10. G. A. Lawrance, Introduction to Coordination Chemistry, John Wiley & Sons Ltd, 2010.
11. C.E. Housecroft, A. G. Sharpe, Inorganic Chemistry, Pearson, 2012.

Course	Details				
Code	CH1922106				
Title	**ORGANIC REACTION MECHANISMS**				
Degree	M.Sc.				
Branch(s)	Chemistry				
Year/Semester	1/II				
Type	Core Course				
Credits	4	**Hrs/Week**	4	**Total Hours**	72

CO No.	**Expected Course Outcomes** *Upon completion of this course, the students will be able to:*	Cognitive Level	PSO No.
1	To understand organic reaction mechanisms and to analyse reactions	An	1
2	To study about the reactive intermediates and the rearrangements involved	An	3
3	Describe the chemistry of carbonyl compounds	C	2
4	Learn, Analyse and Apply Concerted Reactions	C	4

PSO – Programme Specific Outcome; CO-Course Outcome; Cognitive Level: R-Remember; U-Understanding; Ap-Apply; An-Analyze; E-Evaluate; C-Create.

Module	Course Description	Hrs	CO No.
1.0	**Organic Reaction Mechanisms and Carbanions**	**18**	
1.1	Review of organic reaction mechanisms with special reference to nucleophilic and electrophilic substitution at aliphatic carbon (SN1, SN2, SNi, SE 1, SE2), elimination (E1 and E2) and addition reactions (regioselectivity: Markovnikov's addition-carbocation mechanism, anti-Markovnikov's addition-radical mechanism). Elimination vs substitution.	6	1
1.2	A comprehensive study on the effect of substrate, reagent, leaving group, solvent and neighbouring group on nucleophilic substitution(SN2 and SN1) and elimination (E1 and E2) reactions.	3	1
1.3	Formation, structure and stability of carbanions; Reactions of carbanions: C-X bond (X = C, O, N) formations through the intermediary of carbanions. Chemistry of enolates and enamines. Kinetic and Thermodynamic enolates- lithium and boron enolates in aldol and Michael reactions, alkylation and acylation of enolates.	2	1
1.4	Nucleophilic additions to carbonyls groups: Name reactions under carbanion chemistry-mechanism of Claisen, Dieckmann, Knoevenagel, Stobbe, Darzen and acyloin condensations, Shapiro reaction and Julia elimination. Favorski rearrangement.	5	1
1.5	Ylids: chemistry of phosphorous and sulphurylids - Wittig and related reactions, Peterson olefination.	2	1

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2.0	**Chemistry of Carbocations and Free Radicals**	**18**	
2.1	Formation, structure and stability of carbocations. Classical and non-classical carbocations. C-X bond (X = C, O, N) formations through the intermediary of carbocations. Molecular rearrangements including Wagner-Meerwein, Pinacol-pinacolone, Semi-pinacol, Dienone-phenol and Benzilic acid rearrangements, Noyori annulation, Prins reaction. C-C bond formation involving carbocations: Oxymercuration, Halolactonisation.	9	2
2.2	Generation of radical intermediates and its (a) addition to alkenes, alkynes (inter and intramolecular) for C-C bond formation - Baldwin's rules (b) fragmentation and rearrangements - Hydroperoxide: formation, rearrangement and reactions. Autooxidation. Name reactions involving radical intermediates: Barton deoxygenation and decarboxylation, McMurry coupling	9	1,2
3.0	**Carbenes, Carbenoids, Nitrenes and Arynes**	**9**	
3.1	Structure of carbenes (singlet and triplet), Generation of carbenes, Addition and Insertion reactions.	2	2
3.2	Reactions of carbenes such as Wolff rearrangement, Reimer-Tiemannreaction. Reactions of ylides by carbenoid decomposition	2	2
3.2	Structure, generation and reactions of nitrene and related electron deficient nitrene intermediates. Hoffmann, Curtius, Lossen, Schmidt and Beckmann rearrangement reactions.	2	2
3.3	Arynes: Generation, structure, stability and reactions. Orientation effect - amination of haloarenes	3	2
4.0	**Chemistry of Carbonyl Compounds**	**9**	
4.1	Reactions of carbonyl compounds: Oxidation, reduction (Clemmensen and Wolf-Kishner), addition (addition of cyanide, ammonia, alcohol) reactions, Aldol condensation, Cannizzaro reaction, Addition of Grignard reagent. Structure and reactions of α, β- unsaturated carbonyl compounds involving electrophilic and nucleophilic addition - Michael addition, Mannich reaction, Robinson annulation.	9	3
5.0	**Concerted Reactions**	**18**	
5.1	Classification - electrocyclic, sigmatropic, cycloaddition, chelotropic,ene and dyotropic reactions. Woodward Hoffmann rules - Frontier orbital and orbital symmetry correlation approaches - PMO method (for electrocyclic and cycloaddition reactions only).	3	4
5.2	Highlighting pericyclic reactions in organic synthesis such as Claisen, Cope, Wittig, Mislow-Evans and Sommelet-Hauser rearrangements. Diels-Alder and Ene reactions (with stereochemical aspects), dipolar cycloaddition (introductory).	6	4
5.3	Unimolecular pyrolytic elimnination reactions:	9	4

	Cheletropic elimination, decomposition of cyclic azo compounds, β-eliminations involving cyclic transition states such as N-oxides (Cope reaction), Acetates and Xanthates (Chugaeve reaction). Problems based on the above topics		

.**References:**

1. R. Bruckner, Advanced Organic Chemistry: Reaction Mechanism, Academic Press, 2002.
2. F.A. Carey, R.A. Sundberg, Advanced Organic Chemistry, Part B: Reactions and Synthesis, 5thEdn., Springer, 2007.
3. W. Carruthers, I. Coldham, Modern Methods of Organic Synthesis, Cambridge University Press, 2005.
4. J. March, M.B. Smith, March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 6thEdn., Wiley, 2007.
5. A. Fleming, Frontier Orbitals and Organic Chemical Reactions, Wiley, 1976.
6. S. Sankararaman, Pericyclic Reactions-A Text Book, Wiley VCH, 2005.
7. R.T. Morrison, R.N. Boyd, S.K. Bhatacharjee, Organic Chemistry, 7thEdn., Pearson, 2011.
8. J. Clayden, N. Greeves, S. Warren, P. Wothers, Organic Chemistry, Oxford University Press, 2004

Course	Details				
Code	CH1922107				
Title	**CHEMICAL BONDING AND COMPUTATIONAL CHEMISTRY**				
Degree	M.Sc.				
Branch(s)	Chemistry				
Year/Semester	I/II				
Type	Core Course				
Credits	4	**Hrs/Week**	4	**Total Hours**	72

CO No.	**Expected Course Outcomes** *Upon completion of this course, the students will be able to:*	Cognitive Level	PSO No.
1	Understand different approximation techniques used in molecular quantum mechanics	Ap	1, 2
2	Identify and explain the main similarities and differences between computational approaches such as HF (Hartree-Fock), semi-empirical, DFT (Density Functional Theory) and force field methods.	Ap	1, 2
3	Describe and identify the various methods' advantages / disadvantages for simulating/modeling various scientific problems.	Ap	1, 2, 3
4	Understand Quantum Mechanical and principles of Molecular Orbital theory, Hückel Molecular Orbital Theory, Valence bond theory and hybridization	U	1
5	Understand Group theoretical principles of Molecular Orbital theory, Valence bond theory and hybridization	U	1
6	Apply the concept of linear combination of atomic orbitals to produce Molecular Orbitals, Hückel Molecular Orbitals and hybrid orbitals to understand the molecular structure and geometry.	Ap	1, 2, 3

PSO – Programme Specific Outcome; CO-Course Outcome; Cognitive Level: R-Remember; U-Understanding; Ap-Apply; An-Analyze; E-Evaluate; C-Create.

Module	Course Description	Hrs	CO. No.
1.0	**Techniques of Approximation in Quantum Mechanics**	**10**	**1**
1.1	Many-body problem and the need of approximation methods, independent particle model.	2	1
1.2	Variation method: variation theorem with proof	2	1
1.3	illustration of variation theorem using the trial function x(a-x) for particle in a 1D-box and using the trial function e^{-ar} for the hydrogen atom	2	1
1.4	Perturbation method: time-independent perturbation method (non-degenerate case), first order correction to energy, illustration by application to particle in a 1D-box with slanted bottom	3	1
1.5	Perturbation treatment of the ground state of the helium atom.	1	1
2.0	**Computational Chemistry**	**26**	**2,3**

2.1	Introduction to computational chemistry: what you can do with computational chemistry, tools of computational chemistry.	1	2
2.2	Hartree-Fock Self-Consistent Field (HF-SCF) method (Derivation): Pauli's principle, slater determinants, Coulomb and exchange Operators, Fock operator, Roothan-Hall equation.	5	2
2.3	Basis functions, Slater type orbitals (STO), Gaussian type orbitals (GTO), sketches of STO and GTO, Classification of basis sets - minimal, double zeta, triple zeta, split valence, polarization and diffuse basis sets, contracted basis sets, Pople style basis sets and their nomenclature, Hartree-Fock limit.	4	2,3
2.4	Electron correlation, Post Hartree-Fock methods: Qualitative ideas on Configuration Interaction(CI) and Møller Plesset approaches to electron correlation.	5	2,3
2.5	Semi-empirical methods: General introduction to semi-empirical methods: basic principles and terminology.	3	2,3
2.6	Introduction to Density Functional Theory (DFT) methods: Hohenberg-Kohn theorems. Kohn-Sham orbitals. Exchange correlation functional. Local density approximation.	4	2,3
2.7	Molecular mechanics methods: Basic principle, Force fields, potential energy functions, inter and intramolecular interactions, empirical parameters, basic idea of QM/MM methods	4	2,3
3.0	**Computational Chemistry Calculations**	**9**	3
3.1	Potential energy surface: stationary point, transition state or saddle point, local and global minima ,geometry optimisation.	3	3
3.2	Molecular geometry input: cartesian coordinates and Z-matrix. Z-matrix of diatomic mo lecules, non-linear triatomic molecule, linear triatomic molecule, polyatomic molecules like ammonia.	3	3
3.3	Comparison and applications of Ab initio, DFT, Semi-empirical and Molecular mechanics methods.	3	3
4.0	**Chemical Bonding**	**18**	**4,6**
4.1	Brief review of Schrödinger equation for molecules and Born-Oppenheimer approximation. Valence Bond (VB) theory, VB theory of H_2 molecule, singlet and triplet state functions (spin orbitals) of H_2.	4	4,6
4.2	Molecular Orbital (MO) theory, MO theory of H_2^+ ion, MO theory of H_2 molecule, MO treatment of homonuclear diatomic molecules and hetero nuclear diatomic molecules. Comparison of MO and VB theories – ionic terms and configuration interaction. Bond order. Correlation diagrams, non-crossing rule. MOs of diatomic molecules – H_2, Li_2, B_2, C_2, N_2, O_2 and F_2, paramagnetism of O_2.	7	4,6
4.3	Quantum mechanical treatment of sp, sp^2 and sp^3 hybridization. Hückel Molecular Orbital (HMO) theory of ethene, allyl systems, butadiene and benzene. Calculation of charge distributions, bond orders and free valency.	7	4,6
5.0	**Applications of Group Theory in Chemical Bonding**	**9**	**5,6**

5.1	Projection operator, generation of SALCs, transformation properties of atomic orbitals, construction of hybrid orbitals with BF_3, CH_4, PCl_5 as examples. Symmetry adapted linear combinations (SALC) of C_{2v}, C_{2h}, C_3, C_{3v} and D_{3h} point groups. MO diagram for water and ammonia.	9	5,6

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Course Texts:

1. Molecular Quantum Mechanics, Peter Atkins and Ronald Friedman, Oxford University Press, 2005
2. Errol Lewar, Computational Chemistry: Introduction to theory and application of Molecular Quantum Mechanics, Second edition, Springer
3. Attila Szabo and Neil S. Ostlund, Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory, Dover Books in Chemistry, 1996
4. D.A. McQuarrie, Quantum Chemistry, University Science Books, 2008.
5. A.S. Kunju, G. Krishnan, Group Theory and its Applications in Chemistry, PHI Learning, 2010
6. R. Ameta, Symmetry and Group Theory in Chemistry, New Age International, 2013

References:

1. I.N. Levine, Quantum Chemistry, 6th Edn., Pearson Education, 2009.
2. R.K. Prasad, Quantum Chemistry, 3rd Edn., New Age International, 2006.
3. F.A. Cotton, Chemical Applications of Group Theory, 3rd Edn., Wiley Eastern, 1990.
4. V. Ramakrishnan, M.S. Gopinathan, Group Theory in Chemistry, Vishal Publications, 1992.
5. J.H. Jensen, Molecular Modeling Basics, CRC Press, 2010.
6. F. Jensen, Introduction to computational chemistry, 2nd Edn., John Wiley & Sons, 2007.
7. A. Leach, Molecular Modelling: Principles and Applications, 2nd Edn., Longman, 2001.
8. J.P. Fackler Jr., L.R. Falvello (Eds.), Techniques in Inorganic Chemistry: Chapter 4, CRC Press, 2011.
9. C.J. Cramer, Essentials of Computational Chemistry: Theories and Models, 2nd Edn., John Wiley & Sons, 2004.

Course	Details				
Code	CH1922108				
Title	**MOLECULAR SPECTROSCOPY**				
Degree	M.Sc.				
Branch(s)	Chemistry				
Year/Semester	1/II				
Type	Core Course				
Credits	3	**Hrs/Week**	3	**Total Hours**	54

CO No.	**Expected Course Outcomes** *Upon completion of this course, the students will be able to:*	Cognitive Level	PSO No.
1	Understand the concepts of spectroscopy	U	1, 2
2	Analyze the relationship between rotational, vibrational and electronic spectroscopy	An	1, 2, 3
3	Understand and relate the concepts of NMR, EPR and Mossbauer spectroscopy	An	1, 2, 3
4	Comprehend the relationship between quantum mechanics, group theory and spectroscopy	An	1, 2, 3
5	Solve problems based on the theory of various spectroscopic techniques	An	1, 2, 3

PSO – Programme Specific Outcome; CO-Course Outcome; Cognitive Level: R-Remember; U-Understanding; Ap-Apply; An-Analyze; E-Evaluate; C-Create.

Module	Course Description	Hrs	CO. No.
1.0	**Foundations of Spectroscopic Techniques**	**9**	**1,4,5**
1.1	Brief review of Electromagnetic spectrum: nature of radiation, Maxwell's equations in free space and in isotropic nonmagnetic media, wave amplitude, angular frequency, phase, period, wavelength, wavenumber, wave vector, velocity of propagation, Black-body radiation, quantum theory of electromagnetic radiation, wave-particle duality, nature of photon – energy, rest mass, momentum, charge, spin, radiant energy, radiant energy density, radiant flux (power), radiant flux density, radiant intensity and radiance.	3	1,4,5
1.2	Radiation-matter interaction: basic concepts of absorption, emission, transmission, reflection, refraction, dispersion, polarization and scattering, absorption cross section, Einstein's coefficients, signal to noise ratio, natural line width, line broadening factors, Doppler broadening, time-dependent perturbation theory (no proof required) and its consequences in spectroscopy, transition moment integral, symmetry and selection rules, intensity of spectral lines, Born-Oppenheimer approximation, rotational, vibrational and electronic energy levels, radiative and non-radiative transitions, relaxation time.	6	1,4,5
2.0	**Rotational Spectroscopy**	**9**	**1,2,4,5**
2.1	Microwave spectroscopy: classical description of molecular rotation, the rigid diatomic rotor – energy Eigen values and Eigen states, principal moments of inertia and classification	9	1,2,4,5

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	(linear, symmetric tops, spherical tops and asymmetric tops), rotational transitions, selection rules, intensity of rotational lines, relative population of energy levels, derivation of J_{max}, effect of isotopic substitution, calculation of intermolecular distance, general layout and working principle of a microwave spectrometer, spectrum of non-rigid rotors, rotational spectra of polyatomic molecules, Stark effect and its application, nuclear spin and electron spin interaction.		
3.0	**Vibrational Spectroscopy**	**9**	**1,2,4,5**
3.1	Infrared spectroscopy: Morse potential energy diagram, anharmonicity – electrical and mechanical, vibrational term values, fundamentals, overtones and hot bands, determination of force constants, diatomic vibrating rotator, break down of the Born-Oppenheimer approximation, effect of nuclear spin, general layout and working principle of an infrared spectrometer, vibrational spectra of polyatomic molecules, potential energy surfaces, normal modes of vibrations, local modes of vibrations, potential energy functions with more than one minimum, combination and difference bands, Fermi resonance, finger print region and group vibrations, principles of FTIR spectroscopy.	9	1,2,4,5
4.0	**Raman and Electronic Spectroscopy**	**18**	**1,2,4,5**
4.1	Raman spectroscopy: scattering of light, classical theory of Raman spectrum, quantum theory of Raman spectrum, general layout and working principle of a Raman spectrometer, rotational and vibrational Raman spectrum, complementary nature of Raman and IR spectra, group theory and mutual exclusion principle, polarized and depolarized Raman lines, basic principles of resonance Raman spectroscopy.	6	1,2,4,5
4.2	Electronic spectroscopy: classical theory of electronic spectroscopy, quantum theory of electronic spectroscopy, general layouts and working principles of an absorption spectrometer and an emission spectrometer, term symbols, selection rules, oscillator strength of transitions, vibronic transitions, Franck-Condon principle, electronic spectra of polyatomic molecules, $n\text{-}\pi^*$ and $\pi\text{-}\pi^*$ transitions, Jablonski diagram, fluorescence and phosphorescence, free electron model of conjugated systems, bathochromic shift and hypsochromic shifts, theory of solvation and spectral shifts, fluorescence quenching, Förster-resonance energy transfer (FRET) – dipole-dipole approximation, Fermi-Golden rule, rate equation of energy transfer, orientation factor, Dexter energy transfer, electron transfer – Marcus classical and semiclassical theory.	8	1,2,4,5
4.3	Lasers – different types of lasers: solid state lasers – Ti:Sapphire, Nd:YAG and semiconductor lasers, gas lasers – helium-neon, argon ion and N_2 lasers. Cavity modes, continuous wave and pulsed lasers, Q-switching, mode locking, harmonic generation	4	

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	Applications of lasers in spectroscopy: Hyper Raman spectroscopy, stimulated Raman spectroscopy, Coherent Anti-Stokes Raman Spectroscopy (CARS)		
5.0	**Resonance Spectroscopy**	**9**	**1,3,4,5**
5.1	NMR spectroscopy: interaction between nuclear spin and applied magnetic field, nuclear energy levels (Hamiltonian and energy), population of energy levels, Larmor precession, Bloch equations and its solutions, Master equation and its implications, rotating frame of reference, relaxation methods, correlation function, spectral density function, magic angle spinning, chemical shift, theory of spin coupling	5	1,3,4,5
5.2	EPR spectroscopy: electron spin in molecules, interaction with magnetic field, g factor, factors affecting g values, fine structure and hyperfine structure, Kramers' degeneracy, McConnell equation.	3	1,3,4,5
5.3	Mossbauer spectroscopy: working principle, chemical shift, factors determining chemical shift	1	1,3,4,5

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References:

1. C.N. Banwell, E.M. McCash, Fundamentals of Molecular Spectroscopy, 4th Edn., Tata McGraw Hill, 1994.
2. J. M. Hollas, Modern spectroscopy, Wiley, 2014.
3. D. C. Harris, M. D. Bertolucci, Symmetry and Spectroscopy: An Introduction to Vibrational and Electronic Spectroscopy, Dover Books, 1989.
4. Principles of fluorescence spectroscopy, J. R. Lakowicz, Springer, 2006.
5. W. Kemp, NMR in chemistry-A Multinuclear Introduction, McMillan, 1986.
6. H. Friebolin, Basic One- and Two-Dimensional NMR-Spectroscopy, Wiley, 1993.
7. H. Gunther, NMR Spectroscopy, Wiley, 1995.
8. C. H. Mayne, Fundamentals of High Resolution Pulse and Fourier Transform NMR Spectroscopy,Webbook, University of Utah, https://chem.utah.edu/_documents/facilities/nmr/Basic%20NMR%20Frame%20Book.pdf
9. D. N. Sathyanarayana, Introduction to Magnetic Resonance Spectroscopy ESR, NMR, NQR, IK International, 2009.
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11. P.W. Atkins, Physical Chemistry, ELBS,1994.
12. D. A. McQuarrie, J. D. Simon, Physical Chemistry: A Molecular Approach, University Science Books, 1997.
13. O. Svelto, Principles of Lasers, Springer, 2010

Course	Details				
Code	CH1922601				
Title	**INORGANIC CHEMISTRY PRACTICAL-I**				
Degree	M.Sc.				
Branch(s)	Chemistry				
Year/Semester	1/I&II				
Type	Practical				
Credits	3	**Hrs/Week**	3	**Total Hours**	108

CO No.	***Expected Course Outcomes*** *Upon completion of this course, the students will be able to:*	Cognitive Level	PSO No.
1	To identify and differentiate between the different rare earth cations by different analytical methods.	U	1,3
2	Develop advanced laboratory skills used in inorganic synthesis including spectroscopic and analytical techniques for identification and characterization of inorganic molecules.	Ap	2
3	Application of safety and chemical hygiene regulations and practices.	Ap	3

PSO – Programme Specific Outcome; CO-Course Outcome; Cognitive Level: R-Remember; U-Understanding; Ap-Apply; An-Analyze; E-Evaluate; C-Create.

Module	Course Description	Hrs	CO No.
1.0	**Separation and identification of two less familiar metal ions**	**54**	
1.1	Separation and identification of two less familiar metal ions such as Tl, W, Se, Mo, Ce, Th, Ti, Zr, V, U and Li. (Anions which need elimination not to be given. Minimum eight mixtures to be given.)	54	1,2,3
2.0	**Colorimetric estimation of metal ions**	**27**	
2.1	Colorimetric estimation of Fe, Cu, Ni, Mn, Cr, NH_4^+, nitrate and phosphate ions.	27	1,2,3
3.0	**Preparation and characterization of metal complexes**	**27**	
3.1	Preparation and characterization of complexes using IR, NMR and electronic spectra. (a) Tris (thiourea)copper(I) complex (b) Potassium tris (oxalato) aluminate (III). (c) Hexammine cobalt (III) chloride. (d) Tetrammine copper (II) sulphate. (e) Schiff's base complexes of various divalent metal ions.	27	1,2,3

References:

1. A.I. Vogel, G.Svehla, Vogel's Qualitative Inorganic Analysis, 7th Edn., Longman,1996.
2. A.I. Vogel, A Text Book of Quantitative Inorganic Analysis, Longman,1966.
3. I.M. Koltoff, E.B. Sandell, Text Book of Quantitative Inorganic Analysis, 3rd Edn.,McMillian, 1968.
4. V.V. Ramanujam, InorganicSemimicro Qualitative Analysis, The NationalPub.Co., 1974.

Course	Details				
Code	CH1922602				
Title	**ORGANIC CHEMISTRY PRACTICAL-I**				
Degree	M.Sc.				
Branch(s)	Chemistry				
Year/Semester	1/I&II				
Type	Practical				
Credits	3	**Hrs/Week**	3	**Total Hours**	108

CO No.	**Expected Course Outcomes** *Upon completion of this course, the students will be able to*:	Cognitive Level	PSO No.
1	Qualitatively separate the organic components	An	3
2	Provide hands on experience in the preparation of TLC, column chromatography	An	3
3	Develop skills in separating techniques	C	3
4	Acquire advanced knowledge in chemical drawing	C	4

PSO – Programme Specific Outcome; CO-Course Outcome; Cognitive Level: R-Remember; U-Understanding; Ap-Apply; An-Analyze; E-Evaluate; C-Create.

Module	Course Description	Hrs	CO No.
1.0	**PART I**	**27**	
1.1	General methods of separation and purification of organic compounds such as: Solvent extraction Soxhlet extraction Fractional crystallization TLC and Paper Chromatography Column Chromatography Membrane Dialysis	27	1,4
2.0	**PART II**	**54**	
2.1	Separation of Organic binary mixtures by chemical/solvent separation methods	18	3,4
2.2	Separation of organic mixtures by TLC	12	3,4
2.3	Separation/ purification of organic mixtures by column chromatography	14	3,4
2.4	Test for detection of rosin in soaps. Estimation of rosin in soaps	10	3,4
3.0	**PART III**	**27**	
3.1	Drawing the structures of organic molecules and reaction schemes by ChemDraw, Symyx Draw and Chemsketch.	18	1,4
3.2	Draw the structures and generate	9	1,4

	the IR and NMR spectra of the substrates and products in the following reactions: 1. Cycloaddition of diene and dienophile (Diels-Alder reaction) 2. Oxidation of primary alcohol to aldehyde and then to acid 3. Benzoin condensation 4. Esterification of simple carboxylic acids 5. Aldol condensation		

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References:

01. A.I. Vogel, A Textbook of Practical Organic Chemistry, Longman, 1974.
02. A.I. Vogel, Elementary Practical Organic Chemistry, Longman, 1958.
03. F.G. Mann, B.C Saunders, Practical Organic Chemistry, 4th Edn., Pearson Education India, 2009.
04. R. Adams, J.R. Johnson, J.F. Wilcox, Laboratory Experiments in OrganicChemistry, Macmillan, 1979.

Course	Details				
Code	CH1922603				
Title	**PHYSICAL CHEMISTRY PRACTICAL**				
Degree	M.Sc.				
Branch(s)	Chemistry				
Year/Semester	1/I & II				
Type	Practical				
Credits	3	Hrs/Week	4	Total Hours	144

CO No.	**Expected Course Outcomes** *Upon completion of this course, the students will be able to*:	Cognitive Level	PSO No.
1	Interpret data from various experiments, including the construction of appropriate graphs and evaluation of errors.	An	3, 4
2	Quantitatively analyze the extent of adsorption of liquids by solids.	An	1
3	Understand the concept of surface forces in various liquids and the effect of reaction conditions on it.	An	3
4	Apply the terms of phase diagrams in binary and tertiary systems which are used in material science and engineering field.	Ap	1
5	Develop skills in applying the distribution law for various solutes between different appropriate solvent pairs in liquid phase chemical reactions.	C	3
6	Compare and apply theoretical approaches such as HF, MP2, DFT in stimulating various scientific problems and calculating various properties of molecules	C	3

PSO – Programme Specific Outcome; CO-Course Outcome; Cognitive Level: R-Remember; U-Understanding; Ap-Apply; An-Analyze; E-Evaluate; C-Create.

Module	Course Description	Hrs	CO. No.
1.0	**Adsorption**	**12**	**1,2**
1.1	Verification of Freundlich and Langmuir adsorption isotherm: charcoal-acetic acid or charcoal-oxalic acid system.	6	1,2
1.2	Determination of the concentration of the given acid using the isotherms.	6	1,2
2.0	**Surface Tension**	**18**	**1,3**
2.1	Determination of the surface tension of a liquid by a) Capillary rise method b) Drop number method c) Drop weight method	6	1,3
2.2	Determination of parachor values.	6	1,3

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2.3	Determination of the composition of two liquids by surface tension measurements	6	1,3
3.0	**Phase Diagrams**	**24**	**1,4**
3.1	Construction of phase diagrams of simple eutectics.	6	1,4
3.2	. Construction of phase diagram of compounds with congruent melting point: diphenyl amine-benzophenone system.	6	1,4
3.3	Effect of (KCl/succinic acid) on miscibility temperature.	6	1,4
3.4	Construction of phase diagrams of three component systems with one pair of partially miscible liquids.	6	1,4
4.0	**Distribution Law**	**18**	**1,5**
4.1	Distribution coefficient of iodine between an organic solvent and water.	6	1,5
4.2	Distribution coefficient of benzoic acid between benzene and water	6	1,5
4.3	Determination of the equilibrium constant of the reaction $KI + I_2 \leftrightarrow KI_3$	6	1,5
5.0	**Computational Chemistry Experiments**	**72**	**1,5**
5.1	Single point energy calculations	12	1,5
5.2	Geometry optimization calculations	12	1,5
5.3	3. Frequency calculations	12	1,5
5.4	Basis set effects	12	1,5
5.5	Predicting Ionization energy, electron affinity, proton affinity and atomization energies.	12	1,5
5.6	Studying chemical reactions and reactivity	12	1,5

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References:

1. J.B. Yadav, Advanced Practical Physical Chemistry, Goel Publishing House, 2001.
2. G.W. Garland, J.W. Nibler, D.P. Shoemaker, Experiments in Physical Chemistry, 8thEdn., McGraw Hill, 2009.
3. J.B. Yadav, Advanced Practical Physical Chemistry, Goel Publishing House, 2001.
4. G.W. Garland, J.W. Nibler, D.P. Shoemaker, Experiments in Physical Chemistry, 8th Edn., McGraw Hill, 2009.
5. James B. Foresman and Aeleen Frisch, Exploring Chemistry With Electronic Structure Methods: A Guide to Using Gaussian, Gaussian, second edition, 1996
6. Gaussian 09, Revision A.02, M. J. Frisch*et al*.,

SEMESTER III

Course	Details				
Code	CH1923109				
Title	**STRUCTURAL INORGANIC CHEMISTRY**				
Degree	M.Sc.				
Branch(s)	Chemistry				
Year/Semester	2/III				
Type	Core Course				
Credits	4	**Hrs/Week**	4	**Total Hours**	72

CO No.	**Expected Course Outcomes** *Upon completion of this course, the students will be able to*:	Cognitive Level	PSO No.
1	Summarize the knowledge in the advanced areas of solid state chemistry such as structure, reactions and phase transition in solids.	U	1,6
2	Relate the electrical, magnetic and optical properties of inorganic compound to its structures.	Ap	1,5
3	Analyze the synthesis, structure and bonding demonstrated by Inorganic Chains, Rings, Cage and Cluster compounds.	An	4
4	Recognize different types of organometallic polymers	U	2
5	Identify different synthesis methods for various solids,	U	5,6
6	Describe magnetic nanoparticles	U	5

PSO – Programme Specific Outcome; CO-Course Outcome; Cognitive Level: R-Remember; U-Understanding; Ap-Apply; An-Analyze; E-Evaluate; C-Create.

Module	Course Description	Hrs	CO No.
1.0	**Solid State Chemistry**	**18**	
1.1	Structure of solids: Imperfections in solids- line defects and plane defects. Structure of the following compounds - Zinc blende, Wurtzite, Rutile, fluorite, antifluorite, Nickel Arsenide, Perosvskite and Ilmenite. Spinels. Inverse spinel structures.	6	1
1.2	Solid state reactions-diffusion coefficient, mechanisms, vacancy diffusion, thermal decomposition of solid-Type I reactions, Type II reactions.	6	1
1.3	Phase transition in solids: classification of phase transitions-first and second order phase transitions, Martensitic transformations, order-disorder transitions and spinodal decomposition. Kinetics of phase transitions, sintering. Growing single crystals-crystal growth from solution, growth from melts and vapor deposition technique.	6	1
2.0	**Electrical, Magnetic and Optical Properties**	**18**	
2.1	Free electron theory of solids. Band theory of solids-	5	2

	Applications to Transition metal compounds and compounds like NaCl, MgO and fullerenes. Energy bands-conductors and non-conductors, Mechanism of intrinsic and extrinsic semiconductors. Mobility of charge carriers- Hall Effect (derivation required). Piezo electricity, pyroelectricity and ferro electricity-hysteresis.		
2.2	Magnetic properties of transition metal oxides, garnets, spinels, ilmenites and perovskites, magnetoplumbites.	4	2
2.3	Optical properties-photoconductivity, photovoltaic effects, luminescence. Applications of optical properties-phosphors, solid state lasers and solar cells.	4	2
2.4	Conductivity of pure metals. Super conductivity-Type I and Type II superconductors, Meisner effect, BCS theory of superconductivity (derivation not required)-Cooper pairs. High temperature superconductors, super conducting cuprates - YBaCu oxide system. Josephson's Junction, conventional superconductors, organic superconductors, fullerenes, carbon nanotubes and graphenes.	5	2
3.0	**Inorganic Chains, Rings, Cage, Clusters**	**18**	
3.1	Chains - catenation, heterocatenation. Silicones. Zeolites-synthesis, structure and applications. Isopoly acids of vanadium, molybdenum and tungsten. Heteropoly acids of Mo and W. Polythiazil-one dimensional conductors. Infinite metal chains.	5	3
3.2	Rings-topological approach to boron hydrides, Styx numbers. Heterocyclic inorganic ring systems- structure and bonding in phosphorous-sulphur and sulphur-nitrogen compounds. Homocyclic inorganic ring systems-structure and bonding in sulphur, selenium and phosphorous compounds.	5	3
3.3	Synthesis, structure and bonding of cage like structures of phosphorous. Boron cage compounds-Wade Mingos Lauher rules, MNO rule, boranes, carboranes, metallacarboranes. Aluminium, indium and gallium clusters, Cages and clusters of germanium, tin and lead, Cages and clusters of tellurium, Mercuride clusters in amalgams. Medical applications of boron clusters-nucleic acid precursors, DNA binders, application of C2B10 for Drug Design, Nuclear Receptor Ligands Bearing C2B10 Cages.	8	3
4.0	**Organometallic Polymers**	**9**	
4.1	Polymers with organometallic moieties as pendant groups, polymers with organometallic moieties in the main chain, condensation polymers based on ferrocene and on rigid rod polyynes, poly(ferrocenylsilane)s, applications of Poly(ferrocenylsilane)s and related Polymers, applications of Rigid-Rod Polyynes, Polygermanes and Polystannanes polymers prepared by ring opening polymerization, organometallic dendrimers.	9	4

5.0	**Magnetic Nanoparticles and Synthesis of Solids**	**9**	
5.1	Synthesis of Solids: Nucleation, Growth, epitaxy and topotaxy. Methods for the synthesis of MgAl2O4, silica glass, indium tin oxide and their coatings, zeolites and alumina based abrassives, hydrothermal synthesis, intercalation and deintercalation. Preparation of thin films, electrochemical methods, chemical vapour deposition. Synthesis of amorphous silica and diamond films- sputtering and laser ablation.	5	5,6
5.2	Magnetic nanoparticles, superparamagnetism and thin films, applications of magnetic nanoparticles- data storage, Magnetic Resonance Imaging (MRI) and Contrast Enhancement using magnetic nanoparticles, biomedical applications of magnetic nanoparticles.	4	5,6

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References:

1. L.V. Azaroff, Introduction to Solids, Mc Graw Hill, 1984.
2. A.R. West, Solid State Chemistry and its Applications, Wiley-India, 2007.
3. D.K. Chakrabarty, Solid State Chemistry, New Age Pub., 2010.
4. D.M. Adams, Inorganic Solids: An Introduction to Concepts in Solid State Structural Chemistry, Wiley, 1974.
5. C.N.R. Rao, K.J. Rao, Phase Transitions in Solids, McGraw Hill, 2010.
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7. Earnshaw, Introduction to Magnetochemistry, Academic Press, 1968.J.E. Huheey, E.A. Keiter, R.L. Keiter, Inorganic Chemistry Principles of Structure and Reactivity, 4th Edn., Harper Collins College Pub.,1993.
8. F.A. Cotton, G. Wilkinson, C.A. Murillo, M. Bochmann, Advanced Inorganic Chemistry, 6th Edn., Wiley-Interscience,1999.
9. K.F. Purcell, J.C. Kotz, Inorganic Chemistry, Holt-Saunders, 1977.
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11. Matthias Driess, Heinrich Nöth, Molecular Clusters of the Main Group Elements, Wiley-VCH, 2004.
12. Richard J.D. Tilley, Understanding Solids, 2nd edition, Wiley, 2013.
13. G.L. Hornyak, J.J. Moore, H.F. Tibbals, J. Dutta, Fundamentals of Nanotechnology, CRC Press, 2009.
14. Chris Binns, Introduction to nanoscience and nanotechnology, wiley, 2010.
15. Vadapalli Chandrasekhar, Inorganic and organometallic polymers, Springer, 2005.
16. Anthony R. West, Basic Solid State Chemistry, John Wiley and Sons, 1988.

Course	Details				
Code	CH1923110				
Title	**ORGANIC SYNTHESES**				
Degree	M.Sc.				
Branch(s)	Chemistry				
Year/Semester	2/ III				
Type	Core Course				
Credits	4	**Hrs/Week**	4	**Total Hours**	72

CO No.	*Expected Course Outcomes* *Upon completion of this course, the students will be able to*:	Cognitive Level	PSO No.
1	Explain metal and non metal based oxidations of alcohols and alkenes.	An	1
2	Explain catalytic hydrogenation and metal based reductions.	An	2
3	Illustrate Brook rearrangement, Tebbe olefination and various name reactions viz. Nef reaction, Kulinkovich reaction, Ritter reaction, Sakurai reaction, Tishchenko reaction.	Ap	2
4	Discuss Metal mediated C-C and C-X Coupling reactions and Multicomponent reactions like Ugi reaction, Passerini reaction and Biginelli reaction.	E	2
5	Discuss Hydride transfer reagents, oxidation – reduction reactions of aluminium isopropoxide.	E	1
6	Ilustrate Synthesis of five and six membered rings, interconversions,and synthesis of heterocycles.	Ap	2
7	Decide the Protecting agents for various functional groups and to discuss peptide synthesis and SPPS	E	2
8	Design the synthesis pathway of target molecules by Retrosynthetic analysis.	C	2

CO-Course Outcome; Cognitive Level: R-Remember; U-Understanding; Ap-Apply; An-Analyze; E-Evaluate; C-Create.

Module	Course Description	Hrs	CO No.
1.0	**Organic Synthesis via Oxidation and Reduction**	**18**	
1.1	Survey of organic reactions with special reference to oxidation and reduction. Metal based and non-metal based oxidations of (a) alcohols to carbonyls [(Chromium-John's oxidation,Collin's oxidation,Sarrett oxidation),Manganese, aluminium and DMSO(Swernoxidation, Moffatt –Pfitzneroxidation, Kornblumoxidation,Corey-Kim oxidation)] based reagents	3	1
1.2	(b) alkenes to epoxides (peroxides/per acids based)-Sharpless asymmetric epoxidation, Jacobsen epoxidation, Shi epoxidation	2	1

1.3	(c) alkenes to diols (Manganese and Osmium based)- Prevost reaction and Woodward modification	2	1
1.4	(d) alkenes to carbonyls with bond cleavage (Manganese based, ozonolysis)	2	1
1.5	(e) alkenes to alcohols/carbonyls without bond cleavage-hydroboration-oxidation, Wacker oxidation, selenium based allylic oxidation. (f) ketones to ester/lactones- Baeyer-Villiger oxidation.	3	1
1.6	(a) Catalytic hydrogenation (Heterogeneous: Palladium/Platinum/Rhodium and Nickel. Homogeneous: Wilkinson).	3	2
1.8	(b) Metal based reductions- Birch reduction, pinacol formation, acyloin formation (c) Enzymatic reduction using Baker's yeast.	3	2
2.0	**Modern Synthetic Methods**	**18**	
2.1	Baylis-Hillman reaction, Henry reaction, Nef reaction, Kulinkovich reaction, Ritter reaction, Sakurai reaction, Tishchenko reaction. Brook rearrangement. Tebbe olefination.	6	3
2.2	Metal mediated C-C and C-X coupling reactions: Heck, Stille, Suzuki-Miyaura, Negishi, Sonogashira, Nozaki-Hiyama-Kishi, Buchwald-Hartwig, Ullmann and Glaser coupling reactions. Click reactions (Huisgen 1,3-dipolar addition).	9	4
2.3	Multicomponent reactions-Ugi reaction,Passerini reaction and Biginelli reaction.	3	4
3.0	**Synthetic Reagents**	**9**	
3.1	Hydride transfer reagents from Group III and Group IV in reductions - LiAlH4, DIBAL-H, Red-Al, NaBH4 and NaCNBH3, selectrides, trialkylsilanes and trialkyl stannane.	3	5
3.2	Aluminum isopropoxide (oxidation and reduction).	2	5
3.3	Reagents such as NBS, DDQ and DCC.Gilmann reagent. DMAP-Borane, PCC, DEAD(Mitsunobu reaction).	4	5
4.0	**Construction of Carbocyclic and Heterocyclic Ring Systems and Protecting Group Chemistry**	**18**	
4.1	Synthesis of four, five and six-membered rings- Photochemical approaches for the synthesis of four membered rings-oxetanes and cyclobutanes, ketene cycloaddition (inter and intra molecular), Pauson-Khand reaction, Volhardt reaction, Bergman cyclization, Nazarovcyclization,cation-olefin cyclization and radical-olefin cyclization.	3	6
4.2	Inter-conversion of ring systems (contraction and expansion)- Demjenov reaction, Reformatsky reaction. Construction of macrocyclic rings-ring closing metathesis (Grubb's catalyst).	3	6
4.3	Formation of heterocyclic rings: 5-membered ring heterocyclic compounds with one or more than one hetero atom like N, S or O - pyrrole, furan, thiophene, imidazole, thiazole and oxazole.	3	6
4.4	Protection and deprotection of hydroxy, carboxyl, carbonyl, and amino groups. Chemo and regio selective protection and deprotection.	4	7
4.5	Protection and deprotection in peptide synthesis: common protecting groups used in peptide synthesis, protecting groups	5	7

	used in solution phase and solid phase peptide synthesis (SPPS).		
5.0	**Retrosynthetic Analysis**	**9**	
5.1	Basic principles and terminology of retrosynthesis: synthesis of aromatic compounds, one group and two group C-X disconnections; one group C-C and two group C-C disconnections.	3	8
5.2	Amine and alkene synthesis: important strategies of retrosynthesis, functional group transposition, important functional group interconversions.	3	8
5.3	Retrosynthesis of D-luciferin. Functional equivalents and reactivity-Umpolung reaction (Ireland-Claisen rearrangement).	3	8

References:

1. M.B. Smith, Organic Synthesis, 3rdEdn.,Wavefunction Inc., 2010.
2. F.A. Carey, R. I. Sundberg, Advanced Organic Chemistry, Part A and B, 5thEdn., Springer, 2007.
3. S. Warren, P. Wyatt, Organic Synthesis: The Disconnection Approach, 2ndEdn., Wiley, 2008.
4. www.arkat-usa.org(Retrosynthesis of D-luciferin)
5. W. Carruthers, I. Coldham, Modern Methods of Organic Synthesis, 4thEdn., Cambridge University Press, 2004.
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7. R. Noyori, Asymmetric Catalysis in Organic Synthesis, John Wiley & Sons, 1994.
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Course	Details				
Code	CH1923111				
Title	**CHEMICAL KINETICS, SURFACE CHEMISTRY AND PHOTOCHEMISTRY**				
Degree	M.Sc.				
Branch(s)	Chemistry				
Year/Semester	2/III				
Type	Core Course				
Credits	4	**Hrs/Week**	4	**Total Hours**	72

CO No.	**Expected Course Outcomes** *Upon completion of this course, the students will be able to:*	Cognitive Level	PSO No.
1	Understand the fundamental concept of the kinetics of a reaction and its mechanism from various theories	U	1
2	Explain the thermodynamic parameters which are involved in the kinetics of a chemical reactions	An	1, 3
3	Explain the effect of catalyst and its mechanism on the kinetics of a chemical reaction	An	1, 3
4	Explain the fundamental concept of photochemistry	Ap	1, 3
5	Define the fundamental concept of surface reactions and various characterization methods	Ap	1, 3 4

CO-Course Outcome; Cognitive Level: R-Remember; U-Understanding; Ap-Apply; An-Analyze; E-Evaluate; C-Create.

Module	Course Description	Hrs	CO No.
1.0	**Kinetics – Theory, reactions and mechanisms**	**27**	**1,2,3**
1.1	Theories of reaction rates: Collision theory-steric factor, collision cross section, reaction cross section, steric factor, potential energy surfaces, early barrier, late barrier, Conventional transition state theory-Eyring equation. Thermodynamic formulation of the two theories. Contour plots, Thermodynamic formulation of the reaction rates. Significance of $\Delta G^{\neq}$, $\Delta H^{\neq}$ and $\Delta S^{\neq}$. Volume of activation. Effect of pressure and volume on velocity of gas reactions.	7	1,2
1.2	Lindemann-Hinshelwood mechanism, qualitative idea of RRKM theory, slater theory, chain reactions: free radical and chain reactions, decomposition of CH_3OCH_3, CH_3CHO, steady state treatment, kinetics of H_2-Cl_2(thermal, photochemical)and H_2-Br_2reactions (thermal, photochemical), H_2-I_2, Rice-Herzfeld mechanism, branching chains H_2-O_2, cool flames, hydrocarbon combustions , significance of k_1, k_{-1}, k_2 Semonov-Hinshelwood mechanism of explosive reactions, degree of branching, mechanisms of step-growth, ionic and addition polymerization, kinetics of anionic and cationic polymerization.	8	1,2
1.3	Fast reactions: relaxation, flow and shock methods, flash photolysis, NMR and ESR methods of studying fast	5	1,2

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	reactions.		
1.4	Reactions in solution: factors determining reaction rates in solutions, effect of dielectric constant and ionic strength, cage effect, Bronsted-Bjerrum equation, primary and secondary kinetic salt effect, influence of solvent on reaction rates, significance of volume of activation, linear free energy relationship, kinetic isotope effect.	7	1,2
2.0	**Catalysis**	**9**	1,2,3
2.1	Acid-base catalysis: specific and general catalysis, Skrabal diagram, Bronsted catalysis law, prototropic and protolytic mechanism with examples, acidity function.	5	1,2,3
2.2	Enzyme catalysis and its mechanism, Michelis-Menten equation, effect of pH and temperature on enzyme catalysis, Mechanisms of heterogeneous catalysis: unimolecular and bimolecular surface reactions, autocatalysis	4	1,2,3
3.0	**Photochemistry**	**18**	4
3.1	Quantum yield, chemical actinometry, excimers and exciplexes, photosensitization, chemiluminescence, bioluminescence, thermoluminescence, pulse radiolysis, hydrated electrons, photostationary state, dimerization of anthracene, ozone layer in the atmosphere.	9	4
3.2	Quenching of fluorescence and its kinetics, Stern-Volmer equation, concentration quenching, fluorescence and structure, delayed fluorescence, E-type and P-type, effect of temperature on emissions, photochemistry of environment, green house effect	9	4
4.0	**Fundamental aspects of Surface Chemistry**	**12**	**1,2,5**
4.1	Different types of surfaces, thermodynamics of surfaces, Gibbs adsorption equation and its verification, surfactants and micelles, surface pressure and surface potential and their measurements and interpretation.	5	1,5
4.2	Adsorption: The Langmuir theory, kinetic and statistical derivation, multilayer adsorption-BET theory, Use of Langmuir and BET isotherms for surface area determination. Application of Langmuir adsorption isotherm in surface catalysed reactions, the Eley-Rideal mechanism and the Langmuir-Hinshelwood mechanism, flash desorption.	7	1,5
5.0	**Surface Characterization techniques**	**6**	**1,2,5**
5.1	Zeta potential, electro-kinetic phenomena, sedimentation potential and streaming potential, Donnan membrane equilibrium	3	1,2,5
5.2	Surface Enhanced Raman Scattering, surfaces for SERS studies, chemical enhancement mechanism, surface selection rules, spectrum of 2-aminophenol, applications of SERS. Low energy electron diffraction and photoelectron spectroscopy, ESCA and Auger electron spectroscopy, scanning probe microscopy, ion scattering, SEM and TEM in the study of surfaces.	3	1,2,5

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Course Texts:

1. Physical Chemistry;K.J. Laidler,J.H. Meiser 2nd Edn.
2. Physical Chemistry; P.W. Atkins, 8th edition

References:

1. J. Rajaram, J.C. Kuriakose, Kinetics and Mechanisms of Chemical Transformations, Macmillan India, 2000.
2. Kalidas , Chemical Kinetic Methods: Principles of Fast Reaction Techniques and Applications, New Age International, 2005.
3. J.W. Moore, R.G. Pearson, Kinetics and Mechanisms, John Wiley & Sons, 1981.
4. P.W. Atkins, Physical Chemistry, ELBS, 1994.
5. D.A. McQuarrie, J.D. Simon, Physiacl chemistry: A Molecular Approach, University Science Books,1997
6. A.W. Adamson, A.P. Gast, Physical Chemistry of Surfaces, 6th Edn., John Wiley
7. & sons, 1997.
8. K.K. Rohatgi-Mukherjee, Fundamentals of Photochemistry, 2nd Edn., New Age International,1986.
9. G. Aruldhas, Molecular structure and Spectroscopy, PHI Learning, 2007

Course	Details				
Code	CH1923112				
Title	**SPECTROSCOPIC METHODS IN CHEMISTRY**				
Degree	M.Sc.				
Branch(s)	Chemistry				
Year/Semester	2/III				
Type	Core Course				
Credits	3	**Hrs/Week**	3	**Total Hours**	54

CO No.	**Expected Course Outcomes** *Upon completion of this course, the students will be able to*:	Cognitive Level	PSO No.
1	Learn the basic principles of interpret uv-visible, chirooptical, vibrational, 1-D and 2-D NMR and Mass spectroscopy for the structure identification of organic compounds	U	1, 2, 3
2	Analyze and interpret uv-visible, chirooptical, vibrational, 1-D and 2-D NMR and Mass spectral data of organic compounds	U, An	1, 2, 3
3	Evaluate various structural possibilities and arrive at the most logical structure of organic compounds by analysis and interpretation of uv-visible, chirooptical, vibrational, 1-D and 2-D NMR and Mass spectral data.	E	1, 2, 3
4	Identify the structure of organic compounds by analysis and interpretation of uv-visible, chirooptical, vibrational, 1-D and 2-D NMR and Mass spectral data.	U, An, Ap	1, 2, 3

CO-Course Outcome; Cognitive Level: R-Remember; U-Understanding; Ap-Apply; An-Analyze; E-Evaluate; C-Create.

odule	Course Description	Hrs	CO No.
1.0	**Ultraviolet-Visible and Chirooptical Spectroscopy**	**9**	**1,2**
1.1	Energy levels and selection rules, Woodward-Fieser and Fieser-Kuhn rules.	2	1
1.2	Influence of substituent, ring size and strain on spectral characteristics. Solvent effect, Stereochemical effect, non-conjugated interactions.	3	1
1.3	Chiro-optical properties - ORD, CD, plane curves, Cotton effect, octant rule, axial haloketone rule, assignment of configuration of chiral molecules.	3	1
	Problems based on the above topics.	1	2
2.0	**Infrared Spectroscopy**	**9**	**1,2,3**
2.1	Fundamental vibrations, characteristic regions of the spectrum (fingerprint and functional group regions), influence of substituent, ring size, hydrogen bonding, vibrational coupling and field effect on frequency, determination of stereochemistry by IR technique.	7	1
2.2	IR spectra of C=C bonds (olefins and arenes) and C=O bonds.	1	1

2.3	Problems on spectral interpretation with examples.	1	2,3
3.0	**Nuclear Magnetic Resonance Spectroscopy**	**18**	**1,2,3**
3.1	NMR phenomenon, ^{1}H nucleius, Zeeman splitting, RF absorption, Larmor precession, relaxation processes, Chemical shift and shielding/deshielding, factors affecting chemical shift, chemical and magnetic non-equivalence, local diamagnetic shielding and magnetic anisotropy.	4	1
3.2	Spin coupling: Spin coupling and peak splitting pattern, Pascal's triangle, Pople notation - AX, AX_2, AX_3, A_2X_3, AB, ABC, AMX type coupling, first order and non-first order spectra, coupling constant, mechanism of coupling, geminal, vicinal and long range coupling, Dirac model, Karplus curve, quadrupole broadening and decoupling, homoallylic coupling, propargylic coupling, deceptive simplicity, virtual coupling, diastereomeric protons.	6	1
3.3	^{13}C NMR: ^{13}C nucleus, natural abundance, sensitivity, ^{13}C chemical shift and structure correlation, proton coupled ^{13}C spectra, proton decoupled ^{13}C spectra, broad band decoupling, rotating frame of reference, mechanism of heteronuclear decoupling, cross polarization, NOE.	3	1
3.4	Simplification non-first order spectra to first order spectra: shift reagents, spin decoupling and double resonance, off resonance decoupling.	1	1
3.5	2D NMR and COSY, HOMOCOSY and HETEROCOSY – HETCOR and HMQC.	1	1
3.6	Polarization transfer, DEPT, selective Population Inversion, INEPT.	2	1
3.7	Problems on spectral interpretation with examples.	1	2,3
4.0	**Mass Spectrometry**	**9**	**1,2,3**
4.1	Molecular ion: basic principles, ion production methods (EI). Soft ionization methods: SIMS, FAB, CA, MALDI, PD, Field Desorption, Electrospray Ionization. Mass Analyzers: Quadrupole mass spectrometer, Ion trap spectrometer, Time-of-flight mass spectrometer, Fourier-transform spectrometer Isotope abundance, Fragmentation patterns-nitrogen and ring rules. McLafferty rearrangement and its applications.	8	1
4.2	Problems on spectral interpretation with examples.	1	2,3
5.0	**Structural Elucidation Using Spectroscopic Techniques**	**9**	**1,2,3,4**
5.1	Index of hydrogen deficiency, rule of thirteen	1	1
5.2	Identification of structures of unknown organic compounds based on the data from UV-Vis, IR, ^{1}H NMR and ^{13}C NMR spectroscopy (HRMS data or Molar mass or molecular formula may be given).	6	2,3,4
5.3	Interpretation of the given UV-Vis, IR and NMR spectra.	2	2

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References:

1. D.L. Pavia, G.M. Lampman, G.S. Kriz, Introduction to Spectroscopy, 3rd Edn., Brooks Cole, 2000.
2. A.U. Rahman, M.I. Choudhary, Solving Problems with NMR Specroscopy, Academic Press, 1996.
3. L. D. Field, S. Sternhell, J. R. Kalman, Organic Structures from Spectra, 4th Edn., John Wiley & sons, 2007.
4. C.N. Banwell, E.M. McCash, Fundamentals of Molecular Spectroscopy, 4th Edn., Tata McGraw Hill, 1994.
5. D.F. Taber, Organic Spectroscopic Structure Determination: A Problem Based Learning Approach, Oxford University Press, 2007.
6. H. Gunther, NMR Spectroscopy, 2nd Edn., Wiley, 1995.
7. R.M. Silverstein, G.C. Bassler, T.C. Morril, Spectroscopic Identification of Organic Compounds, 5th Edn., Wiley, 1991.
8. D.H. Williams, I. Fleming, Spectroscopic Methods in Organic Chemistry, 6th Edn., McGraw-Hill, 2008.
9. W. Kemp, Organic Spectroscopy, 2nd Edn., Macmillan, 1987.
10. F. Bernath, Spectra of Atoms and Molecules, 2nd Edn., Oxford University Press, 2005.
11. E.B. Wilson Jr., J.C. Decius, P.C. Cross, Molecular Vibrations: The Theory of Infrared and Raman Vibrational Spectra, Dover Pub., 1980.
12. Online spectral databases including RIO-DB.

Course	Details				
Code	**CH1924604**				
Title	**INORGANIC CHEMISTRY PRACTICAL-II**				
Degree	M.Sc.				
Branch(s)	Chemistry				
Year/Semester	2/III&IV				
Type	Practical				
Credits	3	**Hrs/Week**	3	**Total Hours**	54

CO No.	**Expected Course Outcomes** *Upon completion of this course, the students will be able to:*	Cognitive Level	PSO No.
1	To know the various methods used to estimate binary mixtures.	U	1,3
2	Develop laboratory skills in analyzing samples of different alloys like Brass, Bronze, Coin alloy etc and find its composition.	Ap	3
3	Identify different minerals and estimate the percentage of the parent element present in it by suitable analytical methods.	Ap	3
3	Application of safety and chemical hygiene regulations and practices.	Ap	2,3

CO-Course Outcome; Cognitive Level: R-Remember; U-Understanding; Ap-Apply; An-Analyze; E-Evaluate; C-Create.

Module	Course Description	Hrs	CO No.
1.0	**Separation and estimation of two different metal ions**	**54**	
1.1	. Estimation of simple binary mixtures (like Cu-Ni, Cu-Zn, Fe-Cr, Fe-Cu, Fe-Ni,Pb-Ca) of metallic ions in solution by volumetric and gravimetric methods	54	1,2,3
2.0	**Determination of the composition of Alloy**	**27**	
2.1	Analysis of one of the alloys of brass, bronze and solder and estimate the percentage composition.	27	1,2,3
3.0	**Analysis of Ore**	**27**	
3.1	Analysis of one of the ores from hematite, chromite, dolomite, monazite, ilmenite.	27	1,2,3

References:

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

Course	Details				
Code	CH1924605				
Title	**ORGANIC CHEMISTRY PRACTICAL- II**				
Degree	M.Sc.				
Branch(s)	Chemistry				
Year/Semester	2/III&IV				
Type	Practical				
Credits	3	**Hrs/Week**	3	**Total Hours**	54

CO No.	**Expected Course Outcomes** *Upon completion of this course, the students will be able to:*	Cognitive Level	PSO No.
1	Apply the organic synthetic strategies in multi-step synthesis	Ap	1
2	Synthesise organic compounds in atom economy level with less time	An	3
3	Analyze various unknown spectrums	C	2
4	Prepare organic compounds in an environmental friendly way	C	1

CO-Course Outcome; Cognitive Level: R-Remember; U-Understanding; Ap-Apply; An-Analyze; E-Evaluate; C-Create.

Module	Course Description	Hrs	CO No.
1.0	**PART I**	**40**	
1.1	Preparation Involving Two step Synthetic Sequences by Chemical Methods	40	1
2.0	**Part II**	**10**	
2.1	Enzyme/coenzyme catalyzed reactions	10	2, 4
3.0	**Part III**	**10**	
3.1	Preparation Involving Multistep Synthetic Sequences by the Green Alternatives of Chemical Methods	10	4
4.0	**Part IV**	**30**	
4.1	Microwave assisted organic Synthesis	30	2
5.0	**Part V**	**18**	
5.1	Prediction of FTIR, UV-Visible, 1H and 13C NMR spectra of the substrates andproducts at each stage of the products synthesized by the above methods.	18	3

References:

01. A.I. Vogel, a Textbook of Practical Organic Chemistry, Longman, 1974.
02. A.I. Vogel, Elementary Practical Organic Chemistry, Longman, 1958.
03. F.G. Mann and B.C Saunders, Practical Organic Chemistry, 4th Edn. Pearson Education India, 2009.
04. J.R. Adams, J.R. Johnson, J.F. Wilcox, Laboratory Experiments in Organic Chemistry, Macmillan, 1979.
05. V.K ahluwalia, Green Chemistry: Environmentally Benign Reactions, Ane Books, 2009
06. Monograph on green Chemistry Laboratory Experiments, Green chemistry Task Force Committee, DST, 2009

Course	Details				
Code	CH1924606				
Title	**PHYSICAL CHEMISTRY PRACTICAL-II**				
Degree	M.Sc.				
Branch(s)	Chemistry				
Year/Semester	2/ III&IV				
Type	Practical				
Credits	3	**Hrs/Week**	4	**Total Hours**	72

CO No.	**Expected Course Outcomes** *Upon completion of this course, the students will be able to:*	Cognitive Level	PSO No.
1	Determine the rate constant of first and second order reactions.	E	3
2	Examine the influence of ionic strength on rate constant.	Ap	3
3	Determine the concentrations of acid, sugar solutions, and to determine rate constant of inversion of cane sugar in the presence of HCl by polarimetry	E	3
4	Determine the concentrations and molar refractions using refractive index measurements.	E	3
5	Show the complex formation between mercuric iodide and KI by refractometry.	Ap	3
6	Determine viscosities of various liquids and to determine the composition of liquid mixtures	E	3
7	Verify Kendall's equation by viscosity measurements	E	3
8	Determine the concentration of acid, mixture of acids, degree of ionization etc using conductivity experiments and to verify Onsager Equation.	E	3
9	Determine the concentration of acid, mixture of acids, and mixture of halides by potentiometric measurements.	E	3

PSO – Programme Specific Outcome; CO-Course Outcome; Cognitive Level: R-Remember; U-Understanding; Ap-Apply; An-Analyze; E-Evaluate; C-Create.

Module	Course Description	Hrs	CO No.
1.0	**Chemical Kinetics**	**36**	
1.1	Determination of the rate constant of the hydrolysis of ester by NaOH.	8	1
1.2	Determination of Arrhenius parameters.	8	1
1.3	Kinetics of reaction between $K_2S_2O_8$ and KI.	8	1
1.4	Influence of ionic strength on the rate constant of the reaction between $K_2S_2O_8$ and KI.	8	2
1.5	Iodination of acetone in acid medium.	4	1
2.0	**Polarimetry**	**24**	
2.1	Kinetics of the inversion of sucrose in presence of HCl.	8	3

2.2	Determination of concentration of sugar solution.	4	3
2.3	Determination of the concentration of HCl.	8	3
2.4	Determination of the relative strength of acids.	4	3
3.0	**Refractometry**	**18**	
3.1	Identification of pure organic liquids and oils.	2	4
3.2	Determination of molar refraction of pure liquids.	4	4
3.3	Determination of concentration of solutions(KCl-Water,Glycerol-Water)	4	4
3.4	Determination of molar refraction of solids.	4	4
3.5	Study of complex formation between KI and HgI_2 system.	4	5
4.0	**Viscometry**	**18**	
4.1	Determination of viscosity of pure liquids.	2	6
4.2	Verification of Kendall's equation.	4	7
4.3	Determination of the composition of binary liquid mixtures(alcohol-water,benzene-nitrobenzene,toluene-nitrobenzene).	8	6
4.4	Determination of the molecular weight of a polymer(polystyrene in toluene).	4	6
5.0	**Conductivity Measurements**	**26**	
5.1	Verification of Onsager equation.	4	8
5.2	Determination of degree of ionization of weak electrolytes.	4	8
5.3	Determination of Pka value of organic acids.	2	8
5.4	Determination of solubility of sparingly soluble salts.	4	8
5.5	Titration of a mixture of acids against a strong base.	8	8
5.6	Titration of a dibasic acid against a strong base.	4	8
6.0	**Potentiometry**	**22**	
6.1	Determination of single electrode potentials (Cu and Zn).	2	9
6.2	Application of Henderson Equation.	4	9
6.3	Titration of a mixture of acids against a strong base.	4	9
6.4	Determination of end point of a titration using Gran Plot.	4	9
6.5	Determination of the concentrations of a mixture of Cl^- and I^- ions.	8	9

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References:

1. J.B Yadav, Advanced Practical Physical Chemistry, Goel Publishing House, 2001
2. B. Viswanadhan, Practical Physical Chemistry, Viva Pub, 2005.
3. G.W Garland, J.W Nibler, D.P Shoemaker, Experiments in Physical Chemistry,8thEdn, Mc. Graw Hill,2009.

SEMESTER IV

Course	Details				
Code	CH1924301				
Title	**ADVANCED INORGANIC CHEMISTRY**				
Degree	M.Sc.				
Branch(s)	Chemistry				
Year/Semester	2/IV				
Type	Elective				
Credits	4	**Hrs/Week**	5	**Total Hours**	90

CO No.	**Expected Course Outcomes** *Upon completion of this course, the students will be able to:*	Cognitive Level	PSO No.
1	Apply group theory to solve the problems in chemistry.	Ap	1
2	To apply the knowledge of spectroscopy and photochemistry to solve the various problems in chemistry.	Ap	2
3	To understand the scientific revolutions of nanotechnology and to familiarize the classification of nanostructures and to know the applications of nanoparticles in technologically imperative fields.	Ap	2
4	To understand the chemistry of materials and metal organic frame works.	U	2
5	To describe the chemistry of supramolecules.	An	2

PSO – Programme Specific Outcome; CO-Course Outcome; Cognitive Level: R-Remember; U-Understanding; Ap-Apply; An-Analyze; E-Evaluate; C-Create.

Module	Course Description	Hrs	CO No.
1.0	**Applications of Group Theory**	**27**	
1.1	Transformation properties of atomic orbitals	1	1
1.2	Hybridization schemes for sigma and pi bonding with examples.	2	1
1.3	Symmetry Adapted Linear Combination of Atomic orbitals in tetrahedral, octahedral and sandwich complexes- ferrocene. Formation of symmetry adapted group of ligand, MO diagrams.	6	1
1.4	Ligand field theory-splitting of *d* orbitals in different environments(Oh,Td and Square planar) using group theoretical considerations, construction of energy level diagrams,	6	1
1.5	Correlation diagrams, method of descending symmetry, splitting terms for orbitals, energy levels	6	1
1.6	*d-d* transition-selection rules.	2	
1.7	Determination of modes of vibrations in IR and Raman spectra	4	1

	using character tables in C_{2V},C_{4v},D_4h,O_h.		
2.0	**Inorganic Spectroscopic Methods and Photochemistry**	**18**	
2.1	Infrared and Raman Spectroscopy: structural elucidation of coordination compounds containing the following molecules/ions as ligands-NH_3, H_2O, CO, NO, OH−, SO_4^{2-}, CN−, SCN−, NO_2- and X- (X=halogen). Use of isotopes in interpreting and assigning vibrational spectra.	3	2
2.2	Electron Paramagnetic Resonance Spectroscopy: EPR of $d^1$and d^9transition metal ions in cubic and tetragonal ligand fields, evaluation of *g* values and metal hyperfine coupling constants, electron-electron interactions, Multiple Resonance.	3	2
2.3	Mössbauer Spectroscopy: Applications of Mössbauer spectroscopy in the study of Fe(III) complexes. Compound Identification- The interhalogen compound $I_2Br_2Cl_4$, Iron in very high oxidation states – Fe(V) and Fe(VI) nitride complexes.	3	2
2.4	Excited states in transition metal complexes- intra-ligand excited states and meta-centred excited states. Photochemical reactions-substitution and redox reactions of Cr(III), Co(III), Rh(III) and Ru(II) complexes. Manganese-Based Photosystems for the Conversion of Water into Oxygen. Applications-synthesis and catalysis, chemical actinometry and photochromism. Metal-metal multiple bonds. Dissociative photochemistry- ligand loss.	6	2
2.5	Metal complex sensitizers-electron relay, semiconductor supported metal oxide systems, water photolysis, nitrogen fixation and CO_2 reduction, dinitrogen splitting.	3	2
3.0	**Nanomaterials**	**18**	
3.1	Inorganic nanomaterials: General introduction to nanomaterials. Metals and alloys-Synthesis of nanoparticles of gold, silver, rhodium, palladium and platinum. Metal oxides of transition and nontransition elements-SiO_2, TiO_2, ZnO, Al_2O_3, iron oxides and mixed metal oxide nanomaterials. Non-oxide inorganic naomaterials. Porous Silicon nanomaterials-Fabrication and chemical and biological sensing applications.	6	3
3.2	Diversity in nanosystems: self-assembled monolayers on gold-growth process and phase transitions. Gas phase clusters-formation, detection and analysis. Quantum dots- preparation, characterization and applications. Nanoshells-types of systems, characterization and application. Inorganic Nanotubes-Synthetic strategies, structures, properties and applications. Nanocomposites-Natural nanocomposites, polymer nanocomposites, metal and ceramic nanocomposites and clay nanocomposites.	6	3
3.3	Evolving interfaces of nanotechnology-Nanobiotechnology, Nano-biosensors-active and passive cantilever sensors, cantilever sensor for cancer screening. Optical nanosensors – photonic nanosensors, surface plasmon nanosensors, nanoscale optical resonance grids, guided-mode resonace sensors, Nanotechnology for Manipulation of Biomolecules- optical tweezers, dielectrophoresis, biochips, labs on chips, and	6	3

	integrated systems. Nanocatalysts. Nanomedicines- importance of nanomaterials in the pharmaceutical industry and future possibilities for medical nanotechnology, nanoparticles for medical imaging, nanoparticles for targeting cancer cells, nanoencapsulation for drug delivery to tumors.		
4.0	**Chemistry of Materials and metal organic frame works**	**18**	
4.1	Ceramic Structures- mechanical properties, clay products, refractories- characterisation, properties and applications. Non-silicon semiconductors as light emitting diodes, Thermoelectric (TE) Materials, Applications of metals and alloys in hydrogen storage. Inorganic organic hybrid Composites- Sol-gel ceramics, fillers in elastomers, polymer- modified ceramics.	5	4
4.2	Synthetic Strategies for Inorganic Material Design- Direct Combination, Low Temperature Techniques, Combinatorial Synthesis.	4	4
4.3	Introduction, Porous Coordination Polymers- Frameworks with High Surface Area, Lewis Acid Frameworks, Soft Porous Crystals. Design of Metal Organic Frameworks and Design of Functional Metal– Organic Frameworks by Post-Synthetic Modification.	5	4
4.4	Applications of Metal Organic Frameworks- Separation and Purification of Gases by MOFs, Hydrogen Storage, MOFs in the Pharmaceutical World.	4	4
5.0	**Inorganic Supramolecular Chemistry**	**9**	
5.1	Types of Supermolecules, Examples of Inorganic Supermolecules, Synthetic strategies for inorganic super molecules and coordination polymers, Molecular polygons and tubes, Molecular polyhedra.	4	5
5.2	Diamondoid networks, Inorganic crystal engineering using hydrogen bonds, Organometallic Crystal Engineering, Supramolecular Self-Assembly Caused by Ionic Interactions- Hydrocarbyls, Amides and Phosphides.	5	5

References:

01. F.A. Cotton, Chemical Applications of Group Theory, Wiley-Interscience, 1990.
02. V. Ramakrishnan, M.S. Gopinathan, Group Theory in Chemistry, Vishal Pub., 1985.
03. A.S. Kunju, G. Krishnan, Group Theory and its Applications in Chemistry, PHI Learning, 2010
04. K. Nakamoto, IR and Raman Spectra of Inorganic and Coordination Complexes, Part A- Theory and Applications in Inorganic Chemistry, 6th Edn., John Wiley & sons, 1997.
05. R.S. Drago, Physical Methods in Chemistry, Saunders College, 1992.
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14. T. Pradeep, Nano: the Essentials, Tata Mc Graw Hill, 2007.
15. Bradley D. Fahlman, Materials Chemistry, Third Edition, Springer, 2018.
16. Hee-Gweon Woo, Hong Li, Advanced Functional Materials, Springer, 2011.
17. John. N. Lalena, David A. Cleary, Principles of Inorganic Materials Design, Wiley, 2010.
18. David Farrusseng, Metal-Organic Frameworks. Wiley-VCH, 2011.
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20. Wai Kee Li, Gong-Du Zhou, homas Chung Wai Mak, Advanced Structural Inorganic Chemistry, International Union of Crystallography, 2008.
21. Ionel Haiduc, Frank T. Edelman, Supramolecular Organometallic Chemistry, Wiley-VCH, 1999.
22. J. E. Mark, H. R. Allock, R. West, Inorganic Polymers, Second Edition, Oxford University Press, 2005.

Course	Details				
Code	CH1924302				
Title	**ADVANCED ORGANIC CHEMISTRY**				
Degree	M.Sc.				
Branch(s)	Chemistry				
Year/Semester	2/IV				
Type	Elective				
Credits	4	**Hrs/Week**	5	**Total Hours**	90

CO No.	**Expected Course Outcomes** *Upon completion of this course, the students will be able to*:	Cognitive Level	PSO No.
1	Understand supramolecules and their applications	Ap	1
2	Describe green alternatives and stereoselective transformations	An	2
3	Learn the basic concepts of nano chemistry and the role of polymers	C	1
4	To analyse the chemistry of natural products and medicines	An	3
5	Introduction to the methodology of research	U	1

PSO – Programme Specific Outcome; CO-Course Outcome; Cognitive Level: R-Remember; U-Understanding; Ap-Apply; An-Analyze; E-Evaluate; C-Create.

Module	Course Description	Hrs	CO No.
1.0	**Molecular Recognition and Supramolecular Chemistry**	**18**	
1.1	Concept of molecular recognition, host-guest complex formation, forces involved in molecular recognition.	6	1
1.2	Molecular receptors: cyclodextrins, crown ethers, cryptands, spherands, tweezers,carcerands, cyclophanes, calixarenes, carbon nanocapsules.	3	1
1.3	Importance of molecular recognition in biological systems like DNA and protein.Controlled release phenomena.	3	
1.4	Applications of supramolecular complexes in perfumery and medicine. Targeteddrug delivery.	6	1
2.0	**Green Alternatives to Organic Synthesis and Stereoselective transformations**	**18**	
2.1	Principles of Green Chemistry: basic concepts, atom economy, twelve principlesof Green Chemistry, principles of green organic synthesis.	3	2
2.2	Green alternatives to Organic Synthesis: coenzyme catalysed reactions, thiaminecatalyzed benzoin condensation. Green alternatives of molecular rearrangements:pinacol-pinacolone and benzidine rearrangements. Electrophilic aromaticsubstitution reactions. Oxidation-reduction reactions. Clay catalysed synthesis.Condensation reactions. Green photochemical reactions	6	2
2.3	Green Solvents: ionic liquids, supercritical CO2, fluorous chemistry	3	2

2.4	General principles of microwave and ultrasound assisted organic synthesis.	3	2
2.5	Assymmetric induction-chiral auxiliaries and chiral pool.Enantioselective catalytic hydrogenation developed by Noyori and Knowels.Assymetric aldol condensation pioneered by Evans. Assymmetric Diels-Alder reactions. Assymmetric epoxidation using Jacobsen's catalyst	3	2
3.0	**Principles of Nanochemistry and Advances in Polymer Chemistry**	**18**	
3.1	Basic principles of Nanochemistry: methods of synthesis of Nanomaterials (basicidea only). Characterisation of Nanomaterials: UV-Visible spectroscopy, SEM,TEM, STM, XRD (principles only).Applications of nanomaterials in medicine	9	3
3.2	Conducting polymers, polymers for NLO applications, temperature resistant andflame retardant polymers, polymers for medical applications. Dendrimers and dendritic polymers: terminology, classification of dendrimers.Methods of synthesis: convergent and divergent approaches. Dendrimers asnanocapsules. Applications of dendrimers. Hyperbranched polymers: definition, synthesis, applications.	9	3
4.0	**Chemistry of Natural Products and Biomolecules**	**18**	
4.1	Basic aspects of structure and classification of terpenoids,alkaloids, steroids and plant pigments. Nomenclature of prostaglandins.	2	4
4.2	Synthesis of camphor, atropine, papaverine, quinine, cyanin, quercetin,β-carotene, testosterone, PGE2 and PGF2α. Nomenclature of prostaglandins	5	4
4.3	Methods for primary structure determination of peptides, proteins and nucleic acids. Replication of DNA, flow of genetic information, protein biosynthesis, transcription and translation, Genetic code, regulation of gene expression, DNA sequencing. The Human Genome Project. DNA profiling and the Polymerase Chain Reaction (PCR).	4	4
4.4	Biosynthesis of cholesterol, α- terpineol, morphine, glucose and phenyl alanine. Biogenesis of isoprenoids and alkaloids. Biomimetic synthesis of progesterone and sparteine.	7	4
5.0	**Medicinal Chemistry, Drug Designing & Research Methodology**	**18**	
5.1	Introduction to Drug design: modeling techniques, receptor proteins, drugreceptorinteraction, drug action, drug selectivity, drug metabolism.	3	4
5.2	Important chemicals used in drug action, anticoagulants and anticoagulant therapy, anti-anginal drugs, antihypertensive agents, antimalarial drugs,aminoquinolines and alkaloids	6	4
5.3	Antibiotics: Important penicillins, chloramphenicol,	3	4

	tetracyclins and cephalosporins. Drugs for cancer, AIDS and diabetes.		
5.4	The search of knowledge, purpose of research, scientific methods, role of theory,characteristics of research.Types of research: fundamental, applied, historical and experimental research.Chemical literature: primary, secondary and tertiary sources of literature.Classical and comprehensive reference. Literature databases: ScienceDirect,SciFinder. Chemical Abstract. Scientific writing: research reports, thesis, journal articles, books. Types ofpublications: articles, communications, reviews. Important scientific and Chemistry Journals. Impact factor	6	5

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08. A.L. Lehninger, D.L. Nelson, M.M. Cox, Lehninger Principles of Biochemistry, 5th Edn., W.H. Freeman, 2008.
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12. R.L. Dominoswki, Research Methods, Prentice Hall, 1981.
13. J.W. Best, J.V. Kahn, Research in Education, 10th Edn., Pearson/Allyn&Bacon, 2006.
14. H.F. Ebel, C. Bliefert, W.E. Russey, The Art of Scientific Writing, Wiley-VCH, 2004.

Course	Details				
Code	CH1924303				
Title	**ADVANCED PHYSICAL CHEMISTRY**				
Degree	M.Sc.				
Branch(s)	Chemistry				
Year/Semester	2/IV				
Type	Elective				
Credits	4	**Hrs/Week**	4	**Total Hours**	90

CO No.	**Expected Course Outcomes** *Upon completion of this course, the students will be able to*:	Cognitive Level	PSO No.
1	Identify and analyse the type of crystal structure in solids and the behavior of liquid crystals	An	1
2	Describe and analyse the distribution of velocities of various gas molecules and factors affecting them	An	1
3	Solve problems on electrochemical cell parameters, electrochemical active surface area, current and overpotential under given condition	Ap	1 2
4	Understand the theories of instrumental methods available in analytical chemistry	Ap	3
5	To acquaint the student with the advanced techniques in voltammetry, polarography and coulometry	Ap	1, 3

PSO – Programme Specific Outcome; CO-Course Outcome; Cognitive Level: R-Remember; U-Understanding; Ap-Apply; An-Analyze; E-Evaluate; C-Create.

Module	Course Description	Hrs	CO No.
1.0	**Crystallography**	**18**	
1.1	Miller indices, point groups (derivation not expected), translational symmetry, glide planes and screw axes, space groups, simple cases like triclinic and monoclinic systems, interplanar spacing and method of determining lattice types, reciprocal lattices..	5	1
1.2	Methods of characterizing crystal structure, rotating crystal method, powder X-ray diffraction method, determination of structure of sodium chloride by powder method, comparison of the structures of NaCl and KCl, brief outline of single crystal X-ray diffraction and crystal growth techniques.	4	1
1.3	Structure factor: atomic scattering factor, coordinate expression for structure factor, structure by Fourier synthesis.	5	1
1.4	Liquid crystals: mesomorphic state, types, examples and application of liquid crystals. Theories of liquid crystals. Photoconductivity of liquid crystals	4	1
2.0	**Gaseous State**	**9**	
2.1	Derivation of Maxwell's law of distribution of velocities, graphical representation, experimental verification of the law, most probable velocity, derivation of average, RMS and most	6	2

	probable velocities, collision diameter, collision frequency in a single gas and in a mixture of two gases, mean free path, frequency of collision		
2.2	The law of corresponding states, transport properties of gases, effusion, the rate of effusion, time dependence of pressure of an effusing gas	3	2
3.0	**Diffraction Methods, Fluorescence and Atomic Spectroscopic Techniques**	**18**	
3.1	Electron diffraction of gases. Wierl's equation. Neutron diffraction method. Comparison of X-ray, electron and neutron diffraction methods.	3	4
3.2	Fluorescence Spectroscopy: Instrumentation: light source, monochromator, optical filters, photomultiplier tube, polarizers. Fluorescence sensing, mechanism of sensing, sensing techniquesbased on collisional quenching, energy transfer and electron transfer, examples of pH sensors. Novel fluorephores: long life time metal-ligand complexes.	7	4
3.3	Atomic absorption spectroscopy (AAS), principle of AAS, absorption of radiant energy by atoms, classification of atomic spectroscopic methods, measurement of atomic absorption, instrumentation.	3	4
3.4	Atomic emission spectroscopy (AES), advantages and disadvantages of AES, origin of spectra, principle and instrumentation.	3	4
3.5	Flame emission spectroscopy (FES), flames and flame temperature, spectra of metals in flame, instrumentation	2	4
4.0	**Electro Chemistry and Electromotive Force**	**27**	
4.1	Conductance measurements, technique at high frequency and high voltage, results of conductance measurements, ionic mobilities, influence of pressure and temperature on conductance of ions, Walden equations, abnormal ionic conductance.	4	3
4.2	Theories of ions in solution, Drude and Nernst's electrostriction model and Born's model, Debye-Huckel theory, Derivation of Debye-Huckel-Onsager equation, validity of DHO equation for aqueous and non aqueous solutions, Debye- Falkenhagen effect, conductance with high potential gradients, activity and activity coefficients in electrolytic solutions, ionic strength, Debye-Huckel limiting law and its various forms, qualitative and quantitative tests of Debye- Huckel limiting equation, deviations from the DHLL..	8	3
4.3	Osmotic coefficient, ion association, fraction of association, dissociation constant, triple ion and conductance minima, equilibria in electrolytes, association constant, solubility product principle, solubility in presence of common ion, instability constant, activity coefficient and solubility measurement, determination of activity coefficient from equilibrium constant measurement.	4	3
4.4	Electrochemical cells, concentration cells and activity coefficient determination, liquid junction potential, evaluation of thermodynamic properties, the electrode double layer, electrode-electrolyte interface, different	4	3

	models of double layer, theory of multilayer capacity, electrocapillary, Lippmann equation, membrane potential.		
4.5	Fuel cells, classification based on working temperature, chemistry of fuel cells, H_2-O_2 fuel cells.	2	3
4.6	Polarization - electrolytic polarization, dissolution and decomposition potential, concentration polarization, overvoltage, hydrogen and oxygen overvoltage, theories of overvoltage	2	3
4.7	Tafel equation and its significance, Butler-Volmer equation for simple electron transfer reactions, transfer coefficient, exchange current density, rate constants	3	3
5.0	**Electroanalytical Techniques**	**18**	
5.1	Voltametry and polarography: Voltametry-cyclic voltametry, ion selective electrodes, anodic stripping voltametry. Polarography-decomposition potential, residual current, migration current, supporting electrolyte, diffusion current, polarogram, half wave potential, limiting current density, polarograph, explanation of polarographic waves..	5	5
5.2	The dropping mercury electrode, advantages and limitations of DME, applications of polarography, quantitative analysis- pilot ion procedure, standard addition methods, qualitative analysis-determination of half wave potential of an ion, advantages of polarography.	5	5
5.3	Amperometric titrations: general principles of amperometry, application of amperometry in the qualitative analysis of anions and cations in solution, instrumentation, titration procedure, merits and demerits of amperometric titrations.	4	5
5.4	Coulometry: coulometer-Hydrogen Oxygen coulometers, silver coulometer, coulometric analysis with constant current, coulometric tritrations, application of coulometric titrations-neutralization titrations, complex formation titrations, redox titrations. Advantages of coulometry	4	5

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References:

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03. R.J. Silbey, R.A. Alberty, M.G. Bawendi, Physical Chemistry, 4th Edn., Wiley, 2005.
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16. A.I. Vogel, A Text Book of Quantitative Analysis including Instrumental Analysis, John Wiley & Sons, 1961.

Course	Details				
Code	CH1924604				
Title	**INORGANIC CHEMISTRY PRACTICAL - II**				
Degree	M.Sc.				
Branch(s)	Chemistry				
Year/Semester	2/III&IV				
Type	Practical				
Credits	3	**Hrs/Week**	3	**Total Hours**	54

CO No.	**Expected Course Outcomes** *Upon completion of this course, the students will be able to:*	Cognitive Level	PSO No.
1	To know the various methods used to estimate binary mixtures.	U	1,3
2	Develop laboratory skills in analyzing samples of different alloys like Brass, Bronze, Coin alloy etc and find its composition.	Ap	3
3	Identify different minerals and estimate the percentage of the parent element present in it by suitable analytical methods.	Ap	3
3	Application of safety and chemical hygiene regulations and practices.	Ap	2,3

PSO – Programme Specific Outcome; CO-Course Outcome; Cognitive Level: R-Remember; U-Understanding; Ap-Apply; An-Analyze; E-Evaluate; C-Create.

Module	Course Description	Hrs	CO No.
1.0	**Separation and estimation of two different metal ions**	**54**	
1.1	. Estimation of simple binary mixtures (like Cu-Ni, Cu-Zn, Fe-Cr, Fe-Cu, Fe-Ni,Pb-Ca) of metallic ions in solution by volumetric and gravimetric methods	54	1,2,3
2.0	**Determination of the composition of Alloy**	**27**	
2.1	Analysis of one of the alloys of brass, bronze and solder and estimate the percentage composition.	27	1,2,3
3.0	**Analysis of Ore**	**27**	
3.1	Analysis of one of the ores from hematite, chromite, dolomite, monazite, ilmenite.	27	1,2,3

References:

01. A.I. Vogel, A Text Book of Quantitative Inorganic Analysis, Longman, 1966.
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03. G. Pass, H. Sutcliffe, Practical Inorganic Chemistry, Chapman & Hall, 1974.
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Course	Details				
Code	CH1924605				
Title	**ORGANIC CHEMISTRY PRACTICAL- II**				
Degree	M.Sc.				
Branch(s)	Chemistry				
Year/Semester	2/III &IV				
Type	Practical				
Credits	3	**Hrs/Week**	3	**Total Hours**	54

CO No.	**Expected Course Outcomes** *Upon completion of this course, the students will be able to*:	Cognitive Level	PSO No.
1	Apply the organic synthetic strategies in multi-step synthesis	Ap	1
2	Synthesise organic compounds in atom economy level with less time	An	3
3	Analyze various unknown spectrums	C	2
4	Prepare organic compounds in an environmental friendly way	C	1

PSO – Programme Specific Outcome; CO-Course Outcome; Cognitive Level: R-Remember; U-Understanding; Ap-Apply; An-Analyze; E-Evaluate; C-Create.

Module	Course Description	Hrs	CO No.
1.0	**Part I**	**40**	
1.1	Preparation Involving Two step Synthetic Sequences by Chemical Methods	40	1
2.0	**Part II**	**10**	
2.1	Enzyme/coenzyme catalyzed reactions	10	2, 4
3.0	**Part III**	**10**	
3.1	Preparation Involving Multistep Synthetic Sequences by the Green Alternatives of Chemical Methods	10	4
4.0	**Part IV**	**30**	
4.1	Microwave assisted organic Synthesis	30	2
5.0	**Part V**	**18**	
5.0	Prediction of FTIR, UV-Visible, 1H and 13C NMR spectra of the substrates andproducts at each stage of the products synthesized by the above methods.	18	3

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References:

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02. A.I. Vogel, Elementary Practical Organic Chemistry, Longman, 1958.
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Course	Details				
Code	CH1924606				
Title	**PHYSICAL CHEMISTRY PRACTICAL-II**				
Degree	M.Sc.				
Branch(s)	Chemistry				
Year/Semester	2/ III&IV				
Type	Practical				
Credits	3	**Hrs/Week**	4	**Total Hours**	72

CO No.	**Expected Course Outcomes** *Upon completion of this course, the students will be able to:*	Cognitive Level	PSO No.
1	Determine the rate constant of first and second order reactions.	E	3
2	Examine the influence of ionic strength on rate constant.	Ap	3
3	Determine the concentrations of acid, sugar solutions, and to determine rate constant of inversion of cane sugar in the presence of HCl by polarimetry	E	3
4	Determine the concentrations and molar refractions using refractive index measurements.	E	3
5	Show the complex formation between mercuric iodide and KI by refractometry.	Ap	3
6	Determine viscosities of various liquids and to determine the composition of liquid mixtures	E	3
7	Verify Kendall's equation by viscosity measurements	E	3
8	Determine the concentration of acid, mixture of acids, degree of ionization etc using conductivity experiments and to verify Onsager Equation.	E	3
9	Determine the concentration of acid, mixture of acids, and mixture of halides by potentiometric measurements.	E	3

PSO – Programme Specific Outcome; CO-Course Outcome; Cognitive Level: R-Remember; U-Understanding; Ap-Apply; An-Analyze; E-Evaluate; C-Create.

Module	Course Description	Hrs	CO No.
1.0	**Chemical Kinetics**	**36**	
1.1	Determination of the rate constant of the hydrolysis of ester by NaOH.	8	1
1.2	Determination of Arrhenius parameters.	8	1
1.3	Kinetics of reaction between $K_2S_2O_8$ and KI.	8	1
1.4	Influence of ionic strength on the rate constant of the reaction between $K_2S_2O_8$ and KI.	8	2
1.5	Iodination of acetone in acid medium.	4	1
2.0	**Polarimetry**	**24**	
2.1	Kinetics of the inversion of sucrose in presence of HCl.	8	3
2.2	Determination of concentration of sugar solution.	4	3
2.3	Determination of the concentration of HCl.	8	3
2.4	Determination of the relative strength of acids.	4	3

3.0	**Refractometry**	**18**	
3.1	Identification of pure organic liquids and oils.	2	4
3.2	Determination of molar refraction of pure liquids.	4	4
3.3	Determination of concentration of solutions(KCl-Water,Glycerol-Water)	4	4
3.4	Determination of molar refraction of solids.	4	4
3.5	Study of complex formation between KI and HgI_2 system.	4	5
4.0	**Viscometry**	**18**	
4.1	Determination of viscosity of pure liquids.	2	6
4.2	Verification of Kendall's equation.	4	7
4.3	Determination of the composition of binary liquid mixtures(alcohol-water,benzene-nitrobenzene,toluene-nitrobenzene).	8	6
4.4	Determination of the molecular weight of a polymer(polystyrene in toluene).	4	6
5.0	**Conductivity Measurements**	**26**	
5.1	Verification of Onsager equation.	4	8
5.2	Determination of degree of ionization of weak electrolytes.	4	8
5.3	Determination of Pka value of organic acids.	2	8
5.4	Determination of solubility of sparingly soluble salts.	4	8
5.5	Titration of a mixture of acids against a strong base.	8	8
5.6	Titration of a dibasic acid against a strong base.	4	8
6.0	**Potentiometry**	**22**	
6.1	Determination of single electrode potentials (Cu and Zn).	2	9
6.2	Application of Henderson Equation.	4	9
6.3	Titration of a mixture of acids against a strong base.	4	9
6.4	Determination of end point of a titration using Gran Plot.	4	9
6.5	Determination of the concentrations of a mixture of Cl^- and I^- ions.	8	9

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References:

1. J.B Yadav, Advanced Practical Physical Chemistry, Goel Publishing House, 2001
2. B. Viswanadhan, Practical Physical Chemistry, Viva Pub, 2005.
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